

SENSORLAB QUASAR MANUAL

MP MASTER



MA25309

VG QUADRUPOLES

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SENSORLAB INSTRUCTION MANUAL QUASAR

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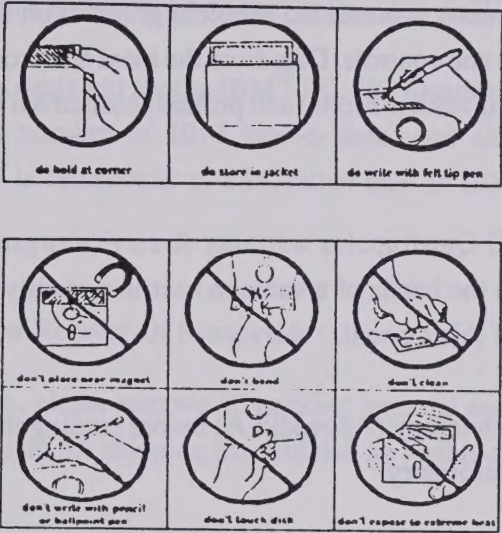
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1. **IMPORTANT SAFETY INFORMATION**

The normal recommendations apply to handling both system and data disks as follows:



WARNING

This mass spectrometer equipment produces high voltages and should be operated and maintained strictly in accordance with its manual.

Servicing should only be undertaken by authorised personnel.

If in doubt contact your local VG Representative.

2. INTRODUCTION

Sensorlab allows control of a Residual Gas Analyser (RGA) from a host PC compatible computer. This is achieved by fitting a VG slot card to the PC computer (which requires at least 512 K RAM and an EGA card to be installed), this connects to a power supply box via a 2.5 m ribbon cable. The power supply box contains all the necessary electronics to drive the RF generator and analyser. Information from the mass spectrometer is presented in colour graphics on the computer, where the user can also alter the RGA settings and controls. Data from the mass spectrometer can also be saved to disk (and looked at later using Data review Mode) and printed / plotted out (if options are installed, see chapter 6).

Sensorlab is backed by the full VG Quadrupoles warranty & service organisation, and brings the latest sophisticated techniques into the hands of a vacuum user in a readily understood and usable form, details are on the last page of this manual.

Study the Glossary of Vacuum Technology (Appendix A) before reading this manual if unfamiliar with vacuum and simple mass spectrometry.

Appendix B contains the full technical details for Sensorlab.

Appendix C describes the general principal of operation with the quadrupole analyser.

Appendix F cover the remote operation of Sensorlab from another host computer over a RS232 type link.

3. INSTALLATION

Sensorlab can be supplied as an upgrade to an existing PC computer or as part of a complete mass spectrometer system from VG Quadrupoles.

The following installation procedure assumes that you have the quadrupole mass spectrometer analyser installed in a vacuum system at a pressure of less than 5×10^{-6} mb.

Although the Sensorlab was designed for the IBM[®] PC, VG Quadrupoles have tested the interface card and software with a number of IBM look-a-likes, and all models have demonstrated compatibility. The text will in future refer to a PC rather than an IBM PC/compatible.

3.1 Checks On Receipt Of Sensorlab

On receipt of your Sensorlab, please remove all packing material and check immediately that you have received all of the items on the shipping list, and that no visible damage has been caused to the package or equipment.

If any damage or omissions are found please report them at once to the company or your local agent.

The packaging for your Sensorlab has been designed to provide all the protection normally required, so should any damage have occurred to the box(es), then please retain it for inspection by us to aid future despatch quality.

3.2 Analyser Head Installation

The analyser head for the Sensorlab instrument is contained inside a plastic envelope. Carefully remove the packaging material from the analyser.

Connect the analyser to your vacuum system using a new copper gasket of the appropriate size. Take care to cross-tighten the bolts to achieve an effective seal. Supplies of gaskets, stainless steel nuts, bolts and washers may be obtained from VG Quadrupoles.

If your vacuum system has a vacuum port flange other than the conflat type, then VG Quadrupoles can supply a special adaptor to interface between the analyser and the port.

CAUTION Great care must be taken not to damage the ceramic insulators whilst inserting the head.

The source of the analyser is of the electron impact type, where electrons are generated by a hot wire filament. Thus the performance of the analyser is affected by the ingress of electrons from any other electron generator in the system if there is a line-of-sight (e.g. B.A. ion gauge).

If the analyser is installed near a magnetic field then the fringe fields (if above 40 gauss) can also effect the performance of the analyser.

Once the analyser is installed, prepare the vacuum system in the usual manner.

The maximum recommended bakeout temperature for the analyser is 300°C. Repeated baking at temperatures above this may cause vacuum leaks to occur on the feedthrough assembly.

3.2.1 Storage of Analysers

Sometimes an analyser is stored at atmospheric pressure for some months before it is installed on a vacuum system. In principle, this is not expected to cause a problem, but please note the following points:-

1. If the analyser gets dusty, its performance will degrade. Keep it in its original wrapping, and stored in a dust-free environment when it is not installed on a vacuum system.
2. Moisture can cause electrical leakage across insulating surfaces. Avoid storing an analyser where extremes of temperature and humidity can occur. Normal office or laboratory conditions are acceptable; an unheated outside store-room is not.
3. Dirt or fingerprints on the 'vacuum' side may cause problems. Avoid touching the analyser directly except the non-vacuum portions of the flange. If it is necessary to handle the inner surface, protection, such as clean gloves or finger tabs should be worn.

3.3 Remote Head Installation

The remote head; for the Sensorlab contains both the RF generator, to provide power to the analyser head, and an amplifier to detect and amplify the ion current arriving at the collector.

The remote head must be guided carefully onto the analyser feedthroughs. The locating slot must align to achieve the correct orientation.

On the 200D and 300D units, the RF generator is connected to the analyser via an integral connecting lead. On the more sensitive gain ranges, the current flowing down this cable from the detector can be as small as 1×10^{-13} Amps. If the cable is knocked or subject to vibration spurious signals are produced which swamp the detector current, causing noisy output. This effect is common to quadrupole RGAs and is called *microphony*; it is due to small emf's generated when the cables are disturbed. It can be minimised by not touching the cables and arranging their path so they can be fastened to a solid fixture.

3.4 Interface Slot Card Installation

1. Remove the cover from the PC computer and unscrew the blanking plate at the rear end of an empty expansion slot, having ensured it is first powered off.
2. Install the interface slot card by locating it over the edge connector and pushing the card firmly into the slot. Ensure that the end furthest from the connector couples into the guide.
3. Secure the interface card by screwing the bracket to the mounting rail at the back lip of the PC.
4. Push the 60-way ribbon cable through the hole created at the back of the PC and attach the connector to the mating plug on the interface slot card.
5. Whilst the cover is off, check that an EGA (Enhanced Graphics Adaptor) is installed and linked to the colour monitor.
6. Fix the PC cover back in position.

3.5 Sensorlab To PC Connection

The Sensorlab unit is suitable for floor standing or for mounting in a 9" rack.

When rack mounted a 1U air gap must be present above and below the unit to provide adequate air flow.

WARNING IF OPERATED WITH THE COVER REMOVED DANGEROUS VOLTAGES MAY BE PRESENT

Instrument Mains Fusing

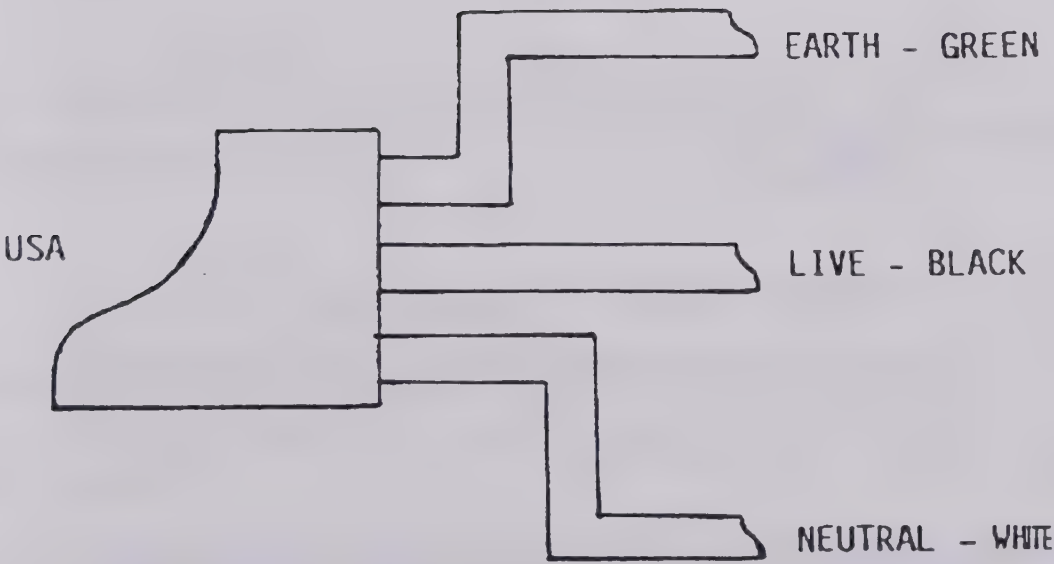
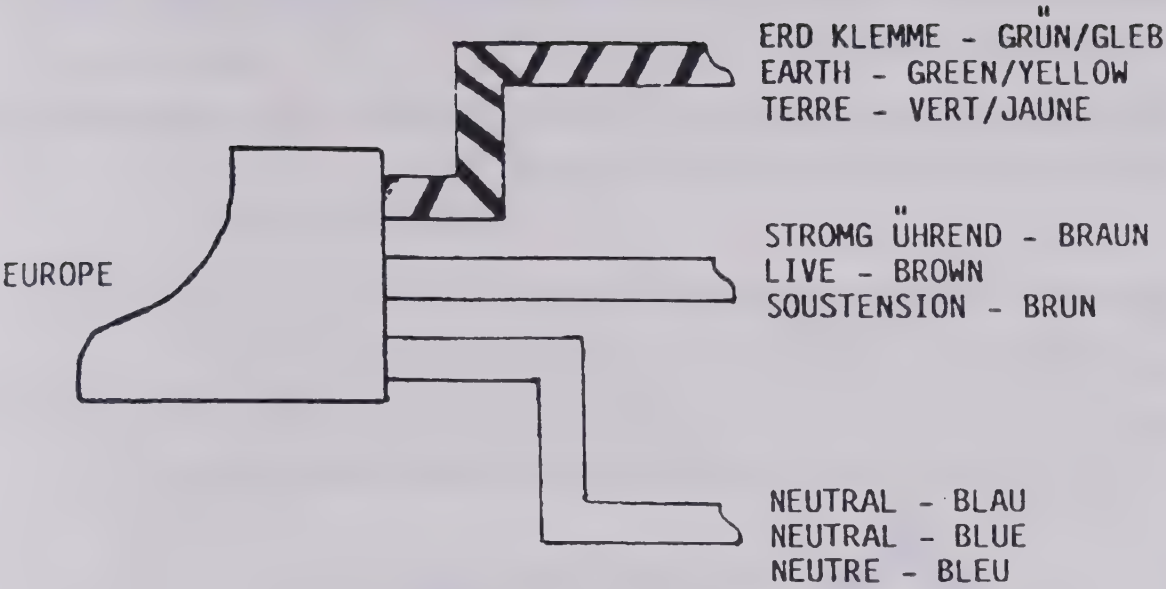
220/240V

1 Amp Anti-surge

100/120V

2 Amp Anti-surge

A mains power lead is supplied with the unit and requires a suitable mains connection. The colour coding of the lead is as shown overleaf:-

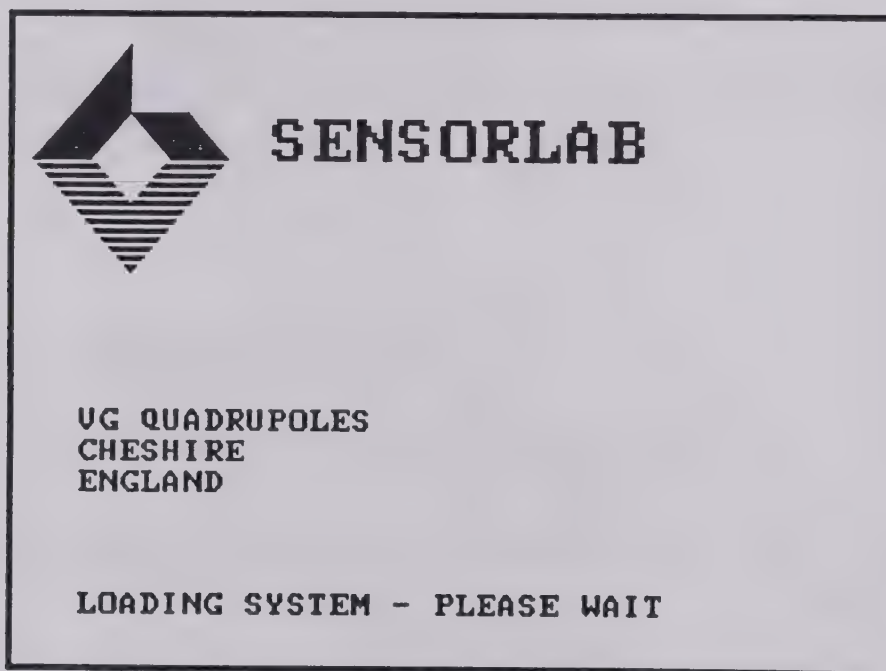


The Sensorlab unit provides the means of linking the mass spectrometer to the PC computer. The 60-way ribbon cable is normally supplied as a flying lead from this unit and connect to the interface card installed on the computer.

Connect the long 37-way cable between the rectangular RF Generator box and the Sensorlab unit, using the screw locks to provide a more reliable connection.

3.6 Getting Going

Place the Sensorlab Start-Up Disk in the floppy disk drive and switch on the PC and the Sensorlab unit.



The data system powers up to display the MASS SPEC CONTROL PAGE so that Emission can be switched on. The 'active' function box (ie, the one whose contents can be changed) is drawn in light blue. As this defaults to the left-hand-side, ie EMISSION, turn Emission on by pressing the **Enter** key.

Press **Esc** to stop the current action or return Sensorlab to the next higher menu level. For example, pressing **Esc** from **MASS SPEC CONTROL PAGE** leads to the **MAIN MENU** of operating modes. Sensorlab is operated by responding to screen prompts. If the baseline box option is unclear press '?' for a help message.

3.6.1 **Hard Disk Installation**

Allow your PC to boot up from the hard disk. Log onto Drive **A:** and type **HDINST**. All the relevant files will be loaded from the floppy disk(s) onto drive **C:** in a sub-directory called **SLABV6**.

If you have a 5¼" disk drive then you will have been provided with two disks. Be sure to insert the **START-UP** disk before typing **HDINST**. As the installation proceeds you will be prompted to insert the **SYSTEM** disk.

To run the software do the following:-

Type : **CD \SLABV6**

Then : **RUN**

The above should be used only once after switching on your PC because the **RUN.BAT** file loads into memory a TSR (terminate and stay resident) program. On subsequent re-runs of the software use **CONTINUE** instead of **RUN**.

3.7 **PC To Quadrupole Matching**

The quadrupole mass spectrometer is supplied with a matching analyser and rf generator. If either of these components are changed, or the analyser is refurbished, it may be necessary to adjust the mass scale alignment.

Do not make any of the adjustments described in this section unless the instrument has been powered on for at least two hours.

3.8 Mass Scale Alignment

View the peak shape and alignment by selecting mode 2 from the Main Menu, Analogue Scan. The mass identification and mark should coincide with the maximum intensity of the relevant peak. The resolution should be such that the valley between adjacent peaks just rises off the baseline. Adjust the mass scale alignment as follows:

1. Ensure that the instrument has been switched on and the mass filter set scanning for at least two hours.
2. Remove the front cover of the rf generator box. Do not loosen any screws on the front panel. The cover is removed by unscrewing the 4 screws at the side of the box.
3. Refer to section later in this Manual which shows the internal layout of the Remote Head.
4. Move the analogue scan window to view a known peak at a high mass (the closer to maximum mass the better). Adjust VR5 'MASS' trimmer so that the peak centre coincides with the relevant mass axis marker.
5. Set Analogue Scan to view the spectrum around the water group (from mass 10 to 20) and adjust VR6 'S' (Scale) so that the mass 12 peak is exactly aligned to the axis marker, with the troughs falling half-way between adjacent scale marks. Use the CURSOR facility to pinpoint the peak centre exactly.
6. Repeat steps 4 and 5 until no further adjustment is necessary.

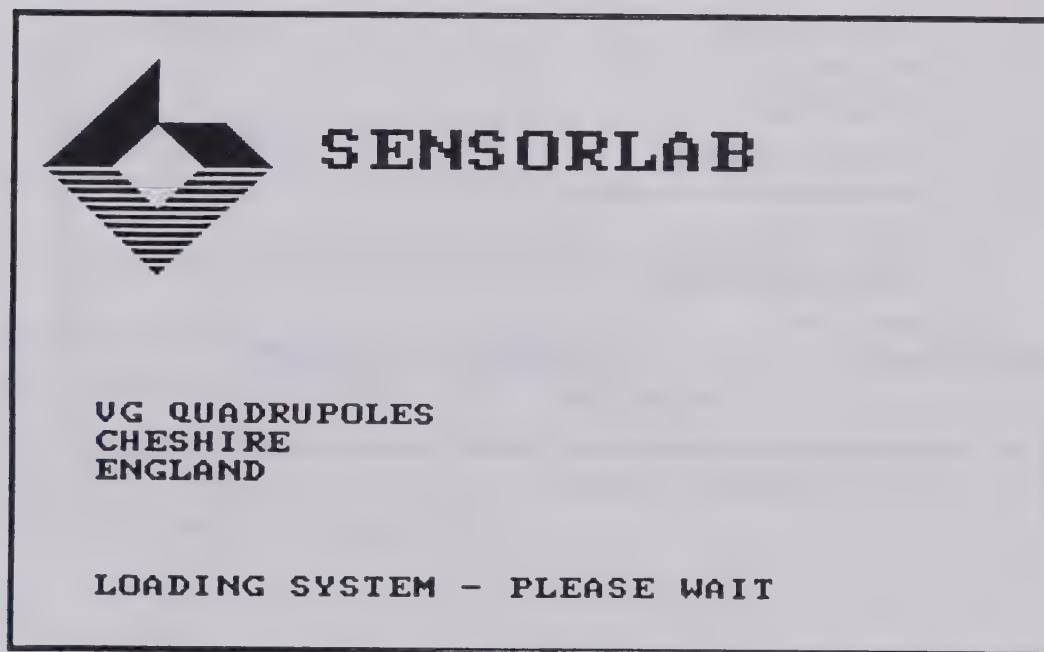
To reset the Resolution use the Analogue Scan mode to adjust VR3 ' ΔM ' at low masses and VR4 'RES' at the higher masses.

4. SOFTWARE DESCRIPTION

This chapter describes in detail each of the software operating modes available from the SENSORLAB. Operation is designed to be simple; use this chapter for reference and be guided through the software by the screen prompts. If in doubt as to which key activates a function, press ? for a helpful message; to clear the message and restore the screen, press any key.

4.1 Initial Program Load

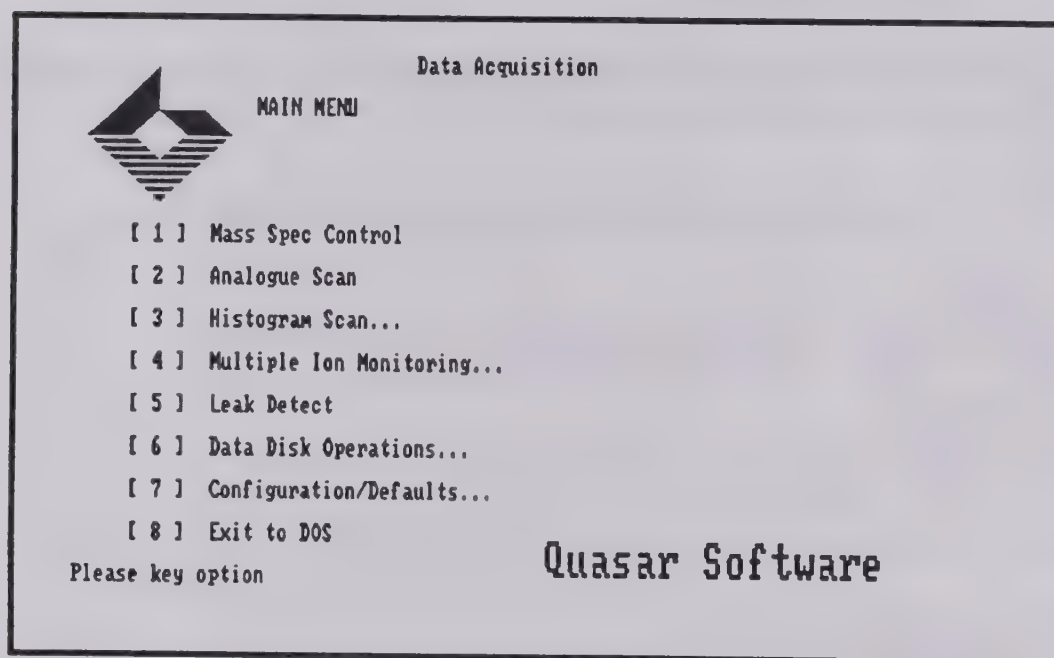
On powering up the PC, it will load its operating system from disk. While the programs are being loaded into memory the banner will be displayed.



If you have a PC that has a 5¼ inch disk drive you require two disks to load this system. First insert the "START-UP DISK" then insert the "SYSTEM DISK" when prompted to do so.

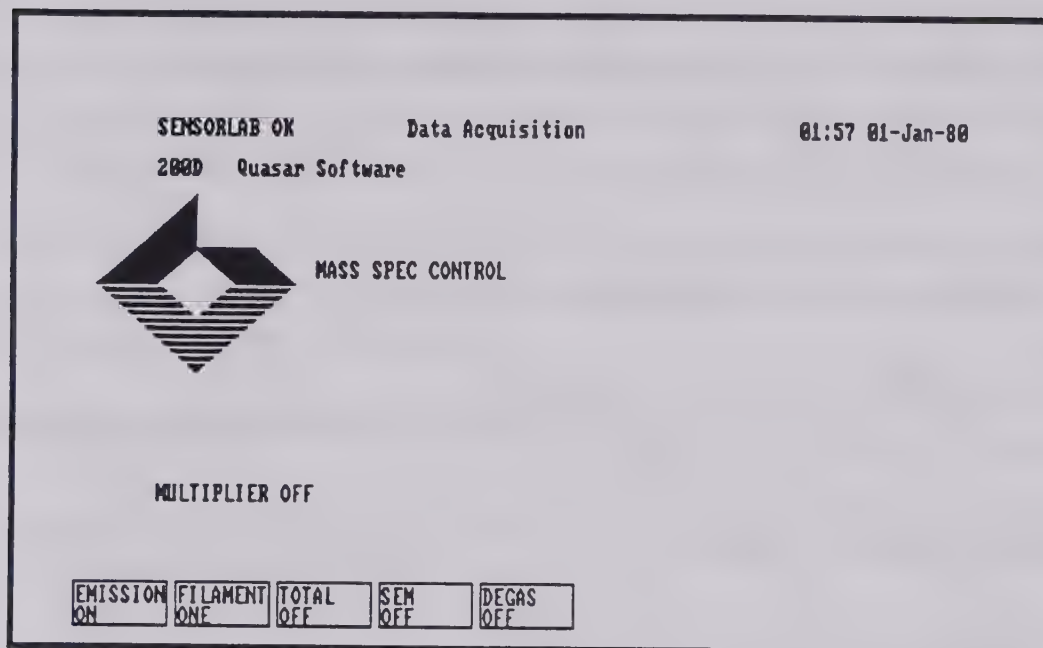
When the system is fully loaded the MASS SPEC CONTROL page is displayed automatically. At this point the user can control various mass spectrometer parameters.

Pressing Esc leads to the main menu:



4.2 Setup Mass Spec

Selecting option 1 of the Main Menu leads to the SETUP MASS SPEC page:



EMISSION is shown as the active function. Press **Ent** to turn emission on and off.

When *EMISSION ON* is selected the message at the top of the screen should show **SENSORLAB OK**, which confirms that all the status lines show normal operation. The data system continuously monitors the status of emission, filament, RF and pressure trip lines and displays an appropriate message if a fault condition arises. For example, turning emission *OFF* produces the message **EMISSION OFF** at the top of the screen.

Use the function boxes to change parameters:

BOX 1 EMISSION

Press **Ent** to switch emission *ON* or *OFF*. When switching emission *ON*, a **WAIT** message is displayed in the box until status is stabilised. If emission cannot be switched on due to a fault condition an error message will be printed accordingly at the top of the screen.

BOX 2 FILAMENT

Press **Ent** to toggle between filament 1 and 2.

BOX 3 TOTAL

Press **Ent** to toggle *TOTAL PRESSURE* read-out *ON* and *OFF*.

BOX 4 SEM

Press **Ent** to toggle the multiplier *ON* or *OFF* (SEM - Secondary Electron Multiplier). When turning the multiplier on the screen clears to display:

measuring total pressure - please wait

which is followed by the multiplier edit page below:

Data Acquisition

SEM CALIBRATION EDIT PAGE

Total Pressure = 0.22F-6

multiplier on [Yes/No]: Yes
volts [600-3500]: 1100
calibration mass (0 for total):
calibrate [Yes/No]: Yes

Enter data in screen format; key **End** to accept; key **Esc** to cancel

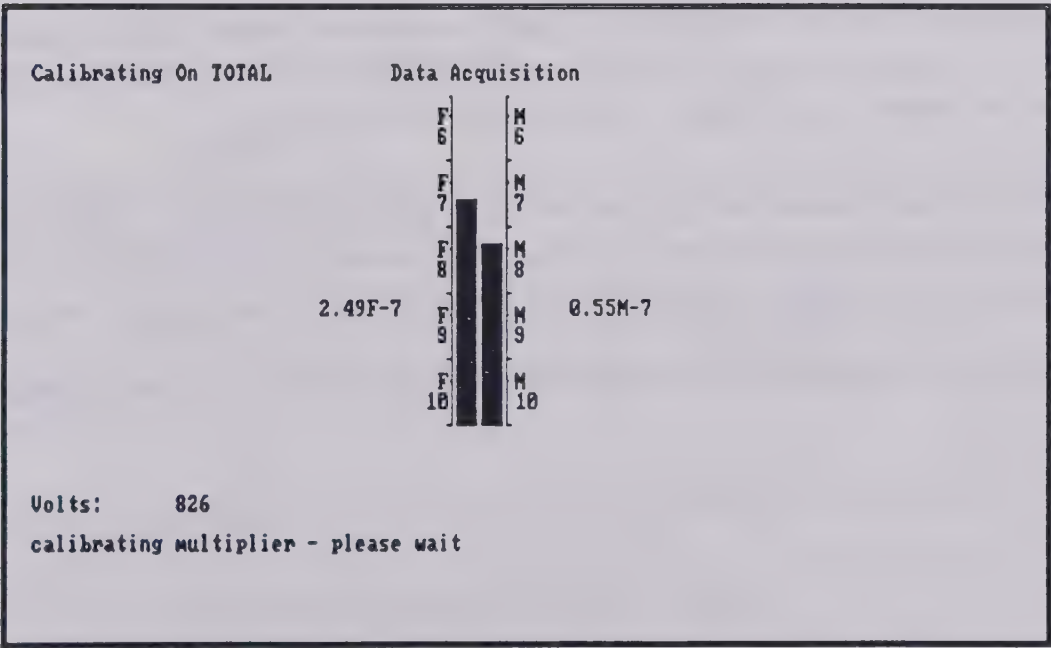
If the measured pressure is below 9.99×10^{-7} mbar, the **multiplier on** field is automatically set to **Yes**. At higher pressures, manually enter **Yes** to turn on the multiplier, but operation at high pressure is not recommended. As a guideline, the highest current drawn from the multiplier must be limited to 1µa.

To calibrate the multiplier against the Faraday detector enter **Yes** next to the **calibrate [Yes/No]** field. To operate the multiplier at a particular voltage, enter **No** after calibrate, and enter the desired voltage after the **volts [600-3500]** field.

The SEM can be calibrated against the Faraday detector in either total or partial pressure mode. To select total pressure enter a value of **0** in the mass box; otherwise enter a mass number on which the SEM will calibrate in partial pressure mode.

When finished, key **End** to execute the options, or **ESC** to abort the mode.

If calibration is not requested, the screen returns to the **SETUP MASS SPEC** page. Otherwise a calibration sequence is initiated as below:



The instrument measures total or partial pressure using the Faraday detector and then displays it as a blue bar. It then increases/decreases the multiplier voltage from the preset value until the same signal reading is obtained. The multiplier reading is plotted as a yellow bar.

The instrument is now calibrated and the screen automatically returns to SETUP MASS SPEC page. The actual voltage set on the SEM is displayed.

If the SEM did not self-calibrate but was enabled at a user defined value, the SEM voltage can still be altered manually. With the SEM on, enable TOTAL pressure by pressing **Ent** over the corresponding base line box, and use the $\uparrow$ and $\downarrow$ keys to alter the SEM voltage in steps of 15V and thus alter the total pressure reading displayed.

The advantage of this is that when the total pressure is too low to be read by the Faraday detector, an external gauge can be used to manually calibrate the SEM.

BOX 5 DEGAS

Degas is a procedure for 'cleaning' the source region of the quadrupole analyser by high energy electron bombardment (500eV). It is used when source contamination is suspected or after a system bakeout to outgas the analyser source area. Only use at pressures below 1×10^{-6} mbar to avoid damage to the source.

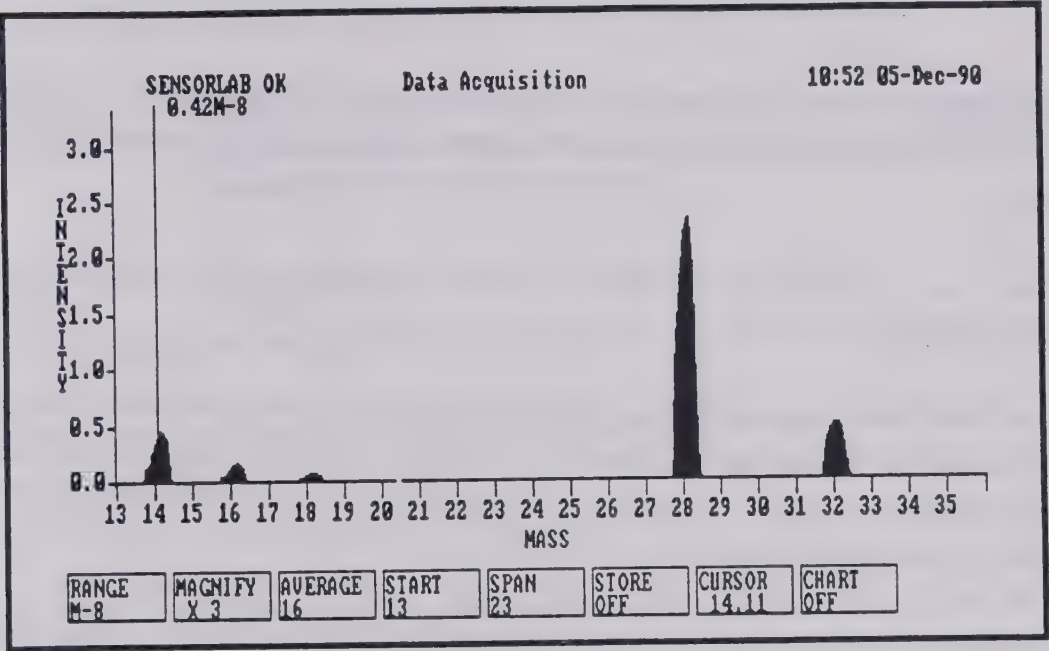
To enable Degas, press **Ent** in the Degas box. A graph is drawn on the screen showing the profile of the degas power ramp against time. As Degas proceeds a thick red line is drawn over the profile line showing the current status of Degas. Pressing **Ent** or **Esc** aborts Degas.

If the SEM is on Degas cannot be used (a screen message to this effect is displayed). Turn the SEM off before any further attempt to use Degas. Likewise, Degas cannot be used if the emission is off. A screen message to this effect is displayed. Turn on the emission before attempting to use Degas.

To exit from the SETUP MASS SPEC Page key **Esc**. This returns the screen to the main menu.

4.3. Analogue Scan

This mode enables the true peak shape and resolution to be viewed throughout the entire mass range. When option 2 is selected from the main menu, an analogue scan is displayed:



Use the function boxes to change parameters:

BOX 1 RANGE

The amplifier gain is increased or decreased using the ↑ and ↓ keys. While the range is being changed the word **change** will appear in the box.

The detector currently in use is indicated by the letters M or F, Multiplier or Faraday respectively. Measurements cannot be made with the Faraday detector if the SEM is turned on (in the SETUP MASS SPEC Page).

The available gain ranges are as follows: Faraday (F): 10^{-5} to 10^{-10} , Multiplier (M): 10^{-7} to 10^{-13} .

Partial pressures are indicated by the peak heights on the display.

BOX 2 MAGNIFY

The display can be magnified by up to a factor of 10 in the y direction. This is achieved by changing the integer value in the magnify box using the ↑ and ↓ keys. Press **Ent** to implement the re-scaling of the y-axis.

BOX 3 AVERAGE

Some signal averaging is performed at the time of measurement to give the best compromise between speed of data collection and signal-to-noise ratio. The *AVERAGE* function allows the user to increase this averaging.

Use the ↑ and ↓ keys to set the desired number of standard measurements to be averaged (powers of two), then press **Ent**.

From the *AVERAGE* box a digital filtering option may be selected. This is selected by using the ↑ key until the word **DIGITAL** appears. Press **Ent** to activate. When this option is selected only one reading at each point is taken. This reading is then passed through a special software algorithm that models a second order low pass filter.

Digital filtering is most useful when fast scans are required but the signal is very noisy. The algorithm is most effective when small mass ranges are selected.

See appendix G for further details on the digital filtering option.

BOX 4 START

This function controls the start of the mass window, the value of which is shown numerically in the box and graphically by a yellow cursor line immediately beneath the spectrum.

The location of the start of the window along the mass axis can be set as desired by using the ↑ and ↓ keys.

Once the desired start mass is indicated, press **Ent** to implement the change.

BOX 5 SPAN

This function controls the span (width) of the mass window, the value of which is shown numerically in the box and graphically by a yellow cursor line, immediately beneath the spectrum.

The mass span can be set as desired by using the ↑ and ↓ keys.

Once the desired mass span is indicated, press **Ent** to implement the change.

NOTE: If either the start or span is changed without pressing **Ent**, the other parameter can also be changed. Pressing **Ent** after that implements the changes made to both parameters.

BOX 6 STORE

This function allows Analogue Scans to be stored to disk for subsequent analysis.

Press **Ent** and the screen clears to display the current list of analogue scan file names. Key **End** to overwrite a file or key **Esc** to create a new file. You will then be prompted for a storage interval. For example, a storage interval of 3 implies that every third scan is stored to disk.

When **STORE** is selected the program determines the amount of free space available on the data disk at the end of each scan. If there is less than 10KB of storage left a warning message will appear. If the data space is exhausted then a message saying **NO SPACE LEFT** will appear. Data storage will then be turned off but scanning will continue.

Each scan is stored to disk until the **STORE** function is turned off by pressing **Ent** again.

BOX 7 CURSOR

This function allows peak positions to be identified. Use the ↑ and ↓ keys to alter the cursor position. The cursor will appear as a vertical red line with the signal value printed at the top.

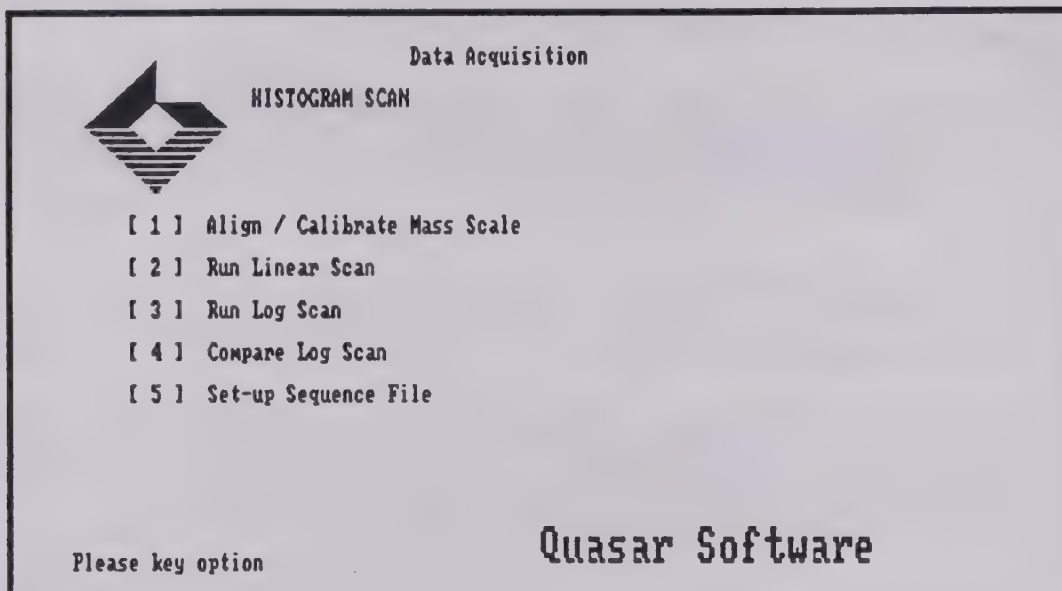
BOX 8 CHART

This function allows the digital to analogue converter which provides the AMU setting to be ramped at its maximum resolution. The optional scan rates of 0.2 AMU/second and 1.0 AMU /second are given. Key **Ent** to activate.

Only one chart scan is done. Chart option is switched off at the end of one scan.

4.4. Histogram Scan

From the *MAIN MENU*, option 3 is the Histogram mode. This has a sub-menu for the five options available from within this mode (as below):



Histogram mode is where a single measurement is taken at each mass. The reading is taken at a position where the peak top is assumed to be. The peak height displayed is the partial pressure at that mass.

If only partial pressure for each mass is required, then this mode has a much faster data acquisition than analogue scan, since only one reading per mass is taken.

4.4.1 Align / Calibrate Mass Scale

If significant drift in the electronics occurs (possibly due to large temperature fluctuations) the single reading at each mass might not be taken at the peak top but on the peak shoulder, causing an inaccurate reading. This option performs a software re-calibration of the mass scale. The software locks onto the peak top for each mass found and interpolates the mass scale for all other masses. Following this histogram readings should be correctly restored to the peak maximum.

If a mass scale alignment has already been performed, alignments can be initiated from the current positions, otherwise the routine uses ideal (theoretical) positions. To leave the edit page, key End.

MASS ALIGNMENT PARAMETERS EDIT PAGE

Initial gain range [7 - 13] : 07

Maximum gain range [7 - 13] : 09

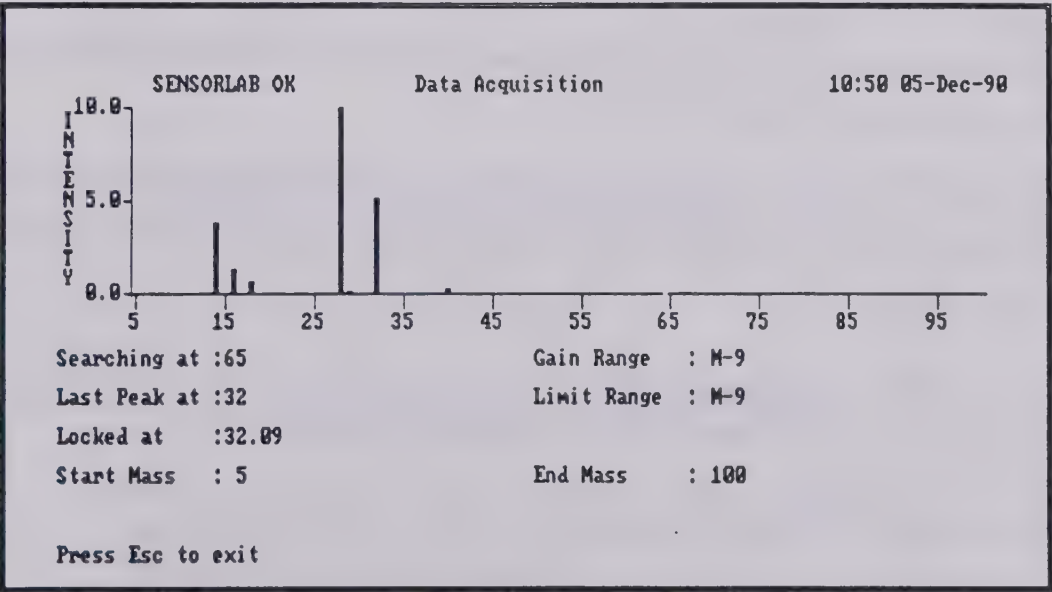
Start Mass for alignment [1 - 200] : 5

End Mass for alignment [1 - 200] : 100

Look from Existing (E) or Ideal (I) mass positions : Ideal

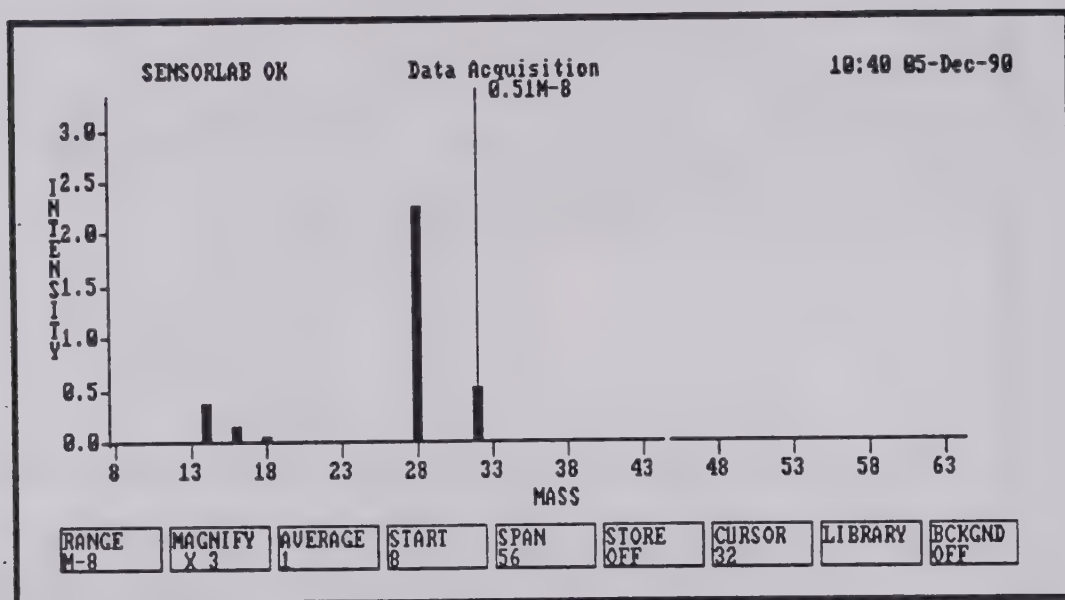
Enter data in screen format; key End to accept; key Esc to cancel

The screen clears to display a real time peak-locking page showing the current status of the parameters. When the alignment is completed (the time taken is dependant on the mass range and pressure ranges chosen) the program returns to the Histogram menu.



4.4.2 Linear Histogram

The second option, linear histogram scan, sets the amplifier on a single but variable fixed-gain range. The screen display below shows a typical linear histogram scan:



Use the function boxes to change parameters:

BOX 1 RANGE

The amplifier gain is increased or decreased using the $\uparrow$ and $\downarrow$ keys. While the range is being changed the word **change** will appear in the box.

The detector currently in use is indicated by the letters **M** or **F**, Multiplier or Faraday respectively. Measurements cannot be made with the Faraday detector if the SEM is on (in the SETUP MASS SPEC page).

The available gain ranges are as follows: Faraday (F): 10^{-5} to 10^{-10} Multiplier (M): 10^{-7} to 10^{-13} . Partial pressures are indicated by the peak heights on the display.

BOX 2 MAGNIFY

The display can be magnified by up to a factor of 10 in the y direction. This is achieved by changing the integer value in the magnify box using the ↑ and ↓ keys. Press **Ent** to implement the re-scaling of the y-axis.

BOX 3 AVERAGE

Some signal averaging is performed at the time of measurement to give the best compromise between speed of data collection and signal-to-noise ratio. The *AVERAGE* function allows the user to increase this averaging.

Digital filtering is not available in histogram mode.

Use the ↑ and ↓ keys to set the desired number of standard measurements to be averaged (powers of two), then press **Ent**.

BOX 4 START

This function controls the start of the mass window, the value of which is shown numerically in the box and graphically by a yellow cursor line immediately beneath the spectrum.

The location of the start of the window along the mass axis can be set as desired by using the ↑ and ↓ keys.

Once the desired start mass is indicated, press **Ent** to implement the change.

BOX 5 SPAN

This function controls the span (width) of the mass window, the value of which is shown numerically in the box and graphically by a yellow cursor line, immediately beneath the spectrum.

The mass span can be set as desired by using the ↑ and ↓ keys.

Once the desired mass span is indicated, press **Ent** to implement the change.

NOTE: If either the start or span is changed without pressing **Ent**, the other parameter can also be changed. Pressing **Ent** after that will implement the changes made to both parameters.

BOX 6 STORE

This function allows Histogram scans to be stored to disk for future analysis.

Press **Ent** and the screen clears to display the current list of histogram scan file names. Key **End** to overwrite a file or key **Esc** to create to create a new fiel. You will then be prompted for a storage interval. For example, a storage interval of 3 implies that every third scan is stored to disk.

When **STORE** is selected the program determines the amount of free space available on the data disk at the end of each scan. If there is less than 10KB of storage left a warning message will appear. If the data space is exhausted then a message will appear saying **NO SPACE LEFT** will appear. Data storage will then be turned off but scanning will continue.

Each scan is stored to disk until the *STORE* function is turned off by pressing **Ent** again.

BOX 7 CURSOR

This function allows peak positions to be identified. Use the $\uparrow$ and $\downarrow$ keys to alter the cursor position. The cursor will appear as a vertical red line with the signal value printed at the top.

BOX 8 LIBRARY

When **Ent** is pressed the instrument prepares to enter the Library mode. The current scan is finished (to get a complete set of up-to-date readings) and then measurements are suspended before going into Library mode.

BOX 9 BACKGROUND

Background mode takes the average of a number of readings at each mass, and then subtracts these readings from all subsequent corresponding pressure readings at the mass they were taken.

The first scan after enabling can be expected to show no peaks. To switch off background subtraction key **Ent** again.

4.4.3 Logarithmic Histogram Display

Choosing option 3 from Histogram sub menu takes the user into the **LOG HISTOGRAM PARAMETERS EDIT PAGE**, where the user sets the decades to be scanned over and the start and end masses for use. The option to store data is also offered at this stage. Once the screen is completed and **End** pressed, the display changes to draw the conventional mass scale, but with a log pressure axis.

LOG HISTOGRAM PARAMETERS EDIT PAGE

lower decade: -9	upper decade: -7
start mass: 5	end mass: 70

Will storage be required? ☐

Enter data in screen format; key End to accept; key Esc to cancel

The software then carries out a single sweep to auto gain-range for the masses selected by the user before drawing in the bars relating to the pressures.

Use the function boxes to change parameters.

BOX 2 LOW AX

Use ↑ and ↓ keys to select the lowest displayed range, key **Ent** to activate this.

BOX 3 HIGH AX

Use ↑ and ↓ keys to select the highest displayed range, key **Ent** to activate.

BOX 4 START

The function controls the start of the mass window, the value of which is shown numerically in the box and graphically by a horizontal yellow cursor immediately beneath the spectrum.

The location of the start of the mass window along the axis can be set using the ↑ and ↓ keys. Key **Ent** to implement the change.

BOX 5 SPAN

This function controls the span (width) of the mass window. The span is selected in a similar way to the **START** mass.

BOX 6 STORE

This box is only accessible if data storage was enabled on the log histogram edit page. Key **enter** in this box to turn the storage off. The storage interval is selected using the ↑ and ↓ keys. Key **Ent** to activate.

BOX 7 CURSOR

This function allows peak positions to be identified. Use the ↑ and ↓ keys to alter the cursor position. The cursor will appear as a vertical red line with the signal value at the top.

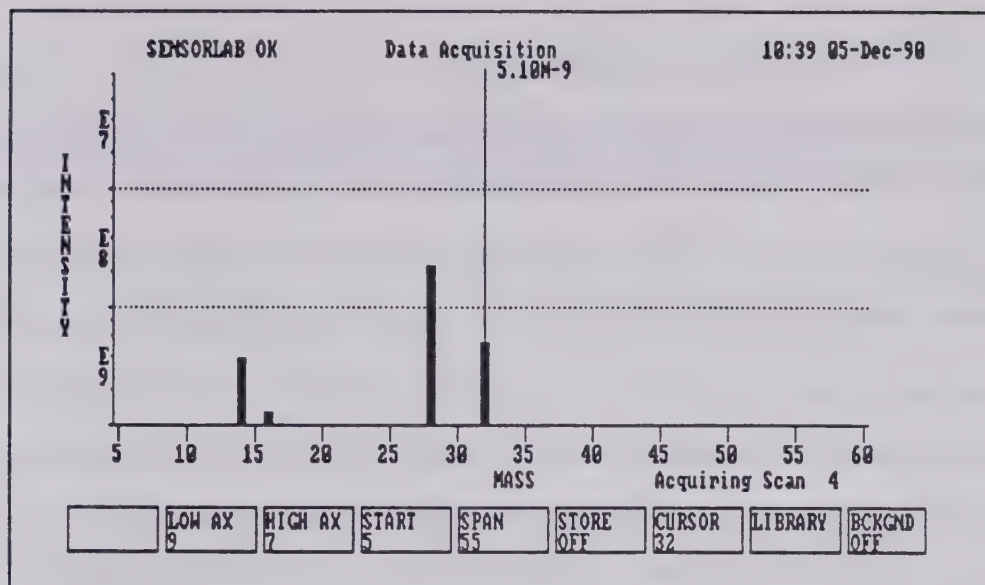
BOX 8 LIBRARY

Key **Ent** to prepare the instrument for library mode. When the current scan is finished the library sub-menu will be displayed.

BOX 9 BACKGROUND

Background mode takes the average of a number of readings at each mass, and then subtracts these readings from all subsequent corresponding pressure readings at the mass they were taken. Thus the first scan after enabling can be expected to show no peaks.

The *AVERAGE* box is no longer available to the user since the program decides how long to spend reading each peak depending on the gain range it has selected for that mass.



4.4.4 Library Mode

Library mode assists the user in the determination of qualitative and quantitative amounts of compounds in mass spectra.

Each molecule has a characteristic mass spectrum. Two processes effect this formation of a mass spectral fingerprint/cracking pattern. Firstly a mass spectrometer measures m/e so that multiple ionisations give mass peaks at $m/2$, $m/3$, $m/4$ etc. The second process arises from fragmentation of the molecule into sub molecular components or atoms.

At the core of the library is a database of up to 200 molecular cracking patterns.

Separate cracking patterns are stored for both faraday and SEM detectors.

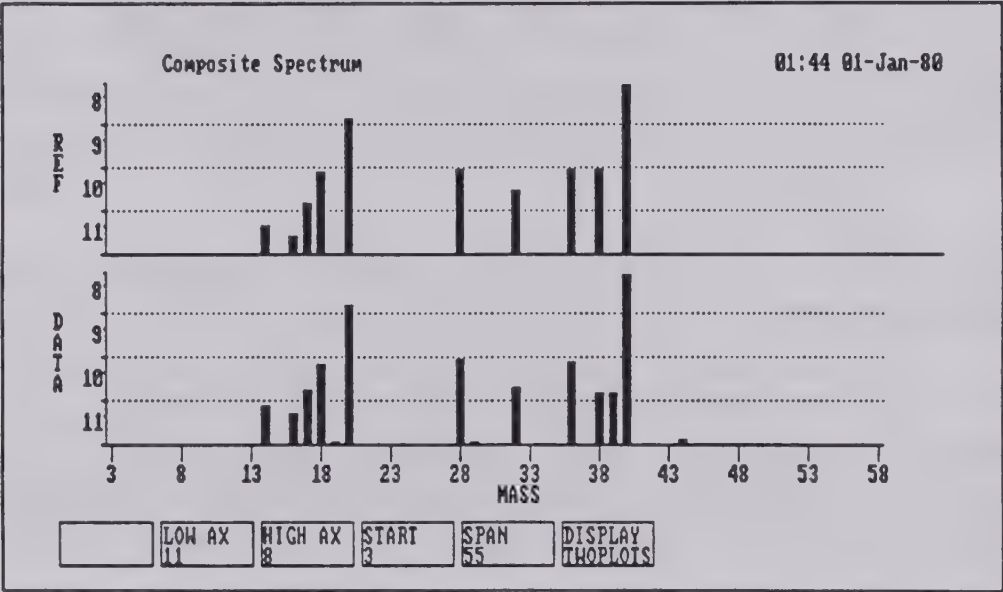
Library mode is entered from either Linear or Logarithmic Histogram mode, and carries forward a real spectrum for analysis. The Library mode also has a sub menu to guide the user through its options.

4.4.4.1 Visual Compare Scan With Library

This mode allows a direct comparison of single database entries against the real histogram spectrum. You are first asked for a library entry number; entering the value 1 will take you to the start of the library.

The reference number (database entry number) for each cracking pattern can be found from option 3.

Key Enter to display the data and selected database cracking pattern in a split screen format.



The reference data is shown in yellow in the top half of the screen, with the file name above the plot. The data is shown in the bottom half, plotted in green.

LOW AX

Use ↑ and ↓ to select the lowest displayed range, key Enter to activate.

HIGH AX

Use ↑ and ↓ to select the highest displayed range, key Enter to activate.

Note : that when LOW AX = HIGH AX a linear axis is displayed.

START

This function controls the start of the mass window, the value of which is shown numerically in the box and graphically by a yellow cursor line immediately beneath the spectrum.

The location of the start of the window along the mass axis can be set as desired by using the ↑ and ↓ keys.

Once the desired start mass is indicated, press Enter to implement the change in the usual way.

SPAN

This function controls the span (width) of the mass window, the value of which is shown numerically in the box and graphically by a yellow cursor line, immediately beneath the spectrum.

The mass span can be set as desired by using the ↑ and ↓ keys.

Once the desired mass span is indicated, press Enter to implement the change.

Note: If either the start or span is changed without pressing Enter, the other parameter can also be changed. Pressing Enter after that will implement the changes made to both parameters.

DISPLAY

Using the ↑ and ↓ keys in this box allow you to select between the various display modes; key Enter to activate that mode.

REF #

This box identifies the current displayed library reference number. Use the ↑ and ↓ keys to step through the library.

4.4.4.2 Automatic Library Search

Automatic library search endeavours to find a list (from 1-20) of gases from the database that best match the data.

The algorithms used are based on statistical and regression techniques and are described in Appendix E. The use of regression techniques allows the estimation of quantitative amounts of material present. The whole library or a subgroup can be used for the search.

On invoking the search the software asks whether you require to search the whole library or just a group.

When you have selected your option, the message started searching... is printed on the screen, and will be followed by a series of stars to show Quasar is progressing through its calculations. When the results have been calculated, they are displayed in tabular mode as percentages.

Use the ↑ and ↓ keys to change between the various display modes.

Very small quantities are specified in ppm (parts per million 1.0ppm = 0.0001%).

Best fit of known compounds is:					18:18 16-Nov-98	
57.74%		of Nitrogen				
38.61%		of Oxygen				
3.64%		of Water				
Correlation is 98.4						
	LOW AX	HIGH AX	START	SPAN	DISPLAY	
	7	7	10	24	TABULAR	

The relative sensitivity is used in the calculation of the percentages. The higher the relative sensitivity the smaller the percentage.

The correlation value displayed represents a goodness of fit. 0% is a poor match and 100% a perfect match.

4.4.4.3 List / Edit Reference Data

This option is used to edit the database of 200 entries.

The library data base is down-loaded from disk and the message 'accessing data file' is flashed on the screen. This leads to the Reference Library Main Menu.

Selecting option 3 from the Reference Library Main Menu leads to the first page of the library data base, which lists 20 cracking patterns:

PAGE NUMBER: 4				
	REFERENCE NAME	FORMULA	MOL WT	P PEAK
61 :	Methylacetate	C3H4(OH)2	74	43
62 :	Hydroxyacetic Acid	C2H(OH)3	76	18
63 :	Fluoroacetone	C3H4(OH)F	76	43
64 :	Fluorobutane	C4H9F	76	43
65 :	Fluoroacetic Acid	C2HF(OH)2	78	18
66 :	Chloropropane	C3H7Cl	78	42
67 :	Benzene	C6H6	78	78
68 :	Chlorofluoroethylene	C2H2FC1	80	45
69 :	Chloroethanol	C2H4(OH)C1	80	31
70 :	Difluoropropane	C3H6F2	80	65
71 :	Trifluoroethylene	C2HF3	82	63
72 :	Chlorofluoroethane	C2H4C1F	82	47
73 :	Cyclohexane	C6H10	82	67
74 :	Krypton	Kr	84	84
75 :	Dichloromethane	CH2C12	84	49
76 :	Trifluoroethane	C2H3F3	84	69
77 :	Cyclohexane	C6H12	84	56
78 :	Freon 22	CHClF2	86	51
79 :	Hexane	C6H14	86	57
80 :		CF4	88	60

Move to entry using cursors; key * to edit entry; key Esc to exit

From left to right the columns are:

REF NO

The library entries are sequentially labelled with a reference number.

REFERENCE NAME

This is the descriptive name of up to 24 characters.

FORMULA

A text representation of the formula, for example water might be put as 'H₂O'.

MOL WT

The molecular weight of the compound. Using the above example of water, this entry would appear as '18'

P PEAK

The mass number of the Principal (major) peak in the cracking pattern for this compound.

The list of cracking patterns are split into pages of 20 entries, with the page number shown in the top right corner. To view the next page key ↓ until the cursor reaches the bottom of the list, key ↓ and the next page is displayed. Users with keyboards can use Pg Dwn and Pg Up to flip between pages. To see the previous page, press the Page Up (Pg Up) or the ↑ key; when the cursor reaches the top of the screen, the previous page will be displayed.

To edit a cracking pattern (or create a new one), move the highlight to the entry you wish to change, using the ↑ and ↓ keys and press End. That database cracking pattern is then shown in a screen editor format:

Name: Ethylene						Reference number: 10			
Formula: C2H4						Principal peak: 28			
Molecular weight: 28						Relative sensitivity (SEM): 1.000			
Relative sensitivity (Faraday): 1.000									
Mass	%	Mass	%	Mass	%	Mass	%	Mass	%
Faraday cracking pattern (ordered by %)									
28	100.000	27	63.000	26	61.000	25	11.000	14	4.000
29	3.000	15	1.000	0	0.000	0	0.000	0	0.000
0	0.000	0	0.000	0	0.000	0	0.000	0	0.000
SEM cracking pattern (ordered by %)									
28	100.000	27	63.000	26	61.000	25	11.000	14	4.000
29	3.000	15	1.000	0	0.000	0	0.000	0	0.000
0	0.000	0	0.000	0	0.000	0	0.000	0	0.000
F7: Copy Faraday to SEM			F8: Copy SEM to Faraday			F9: Order by mass			
End: Accept data			Esc: Cancel edit			F10: Clear data to zeroes			

All the allowable entry fields are shown in blue; the entries in green are for reference only.

The highlight is moved around the screen using the Enter key to move from one field to the next, or using the ↑ and ↓ keys to quickly move up and down the screen.

NAME

Enter a descriptive name of up to 24 characters. Users without keyboard will need to key ? to bring up the single character selection.

FORMULA

Designed for the chemical formula, but any descriptive data (Eg date) up to 16 characters can be entered.

The following additional functions are available from this screen:

F7: Copy Faraday to SEM

This function enables the entered Faraday cracking pattern to be copied to the SEM cracking pattern.

The option is given for a direct copy or a copy with translation. This attempts to account for the difference in SEM detector efficiency by using the graph in figure 3 Appendix D.

F8: Copy SEM to Faraday

This function enables the entered SEM cracking pattern to be copied to the Faraday cracking pattern.

Like the F7 option, the direct copy or copy with translation is available.

F9: Order by Mass/Percentage

The mass/intensity pairs can be displayed in either descending mass or intensity order. If the display is currently ordered by percentage, as in the above example, selecting F9 will change the sequence to be ordered by mass.

F10: Clear data to zeros

Use the F10 function key to initialise all fields on the displayed screen to their default blank state. This is useful if an entry is to be removed from the library.

4.4.4.4 Edit Group

This option allows selection of any library entries for inclusion into sub-groups. These groups may be of any size and the library entries may be placed in any or all of the groups.

On initial entry to this function, i.e. when Quasar has just been installed, there will be no predefined sub-groups. Selecting this option will automatically assume that a new group is to be added. After another group has been created you will, on entry, be presented with a list of available groups to select one for editing.

When the group has been selected you will be shown a list of the current components in that group. To enter a new component into the group type in its cracking pattern formula or the name. The display below shows Neon as the component just added to the group.

```

Editing group # 1, Air
Hydrogen      : H2      : 2
Helium        : He      : 4
Water         : H2O     : 18
Neon          : Ne      : 20
Carbon Monoxide : CO     : 28
Nitrogen      : N2      : 28
Oxygen        : O2      : 32
Argon         : Ar      : 40
Carbon Dioxide : CO2     : 44

Enter chemical formula or name (H2 is different from h2);
key Ent to add the entry to the group list; key Esc to edit Group Name and exit

```

If an exact match for either formula or name is not found in the reference library you are presented with a list of possible entries, i.e. those containing the entered string. The display below shows some of the possible matches, given that just CH was entered.

```

Editing group # 1, Air
No exact match found
with this text, but
text is in these entries:
Methane      : CH4      : 16
Methanol     : CH3OH     : 32
Formic Acid  : CHOOH     : 46
Methylsilane : SiH3CH3   : 46
Chloromethane : CH3Cl     : 50
Difluoromethane : CH2F2     : 52
Chlorofluoromethane : CH2ClF    : 68
Trifluoromethane : CHF3      : 70
Dichloromethane : CH2Cl2    : 84
Freon 22      : CHClF2    : 86
Freon 21      : CHCl2F    : 102

Enter chemical formula or name (H2 is different from h2);
key Ent to add the entry to the group list; key Esc to edit Group Name and exit

```

To select the specific group type in the full identity (formula or name). The display will update to show the new group entries. At this point, as shown in the earlier display, the last entered component is highlighted. Further new components can be added. Keying Escape will change the prompt from entering components to entering/editing the group name. Type in the new group name if required and key Enter. This will return you to the Reference Library Main Menu.

To delete a component from a group; select the group for editing, this will display the current components with the last one highlighted. Deletion removes the highlighted component from the group. By using the ↑ and ↓ keys it is possible to move the highlight to another entry. It should be noted that the deleted reference is then displayed as a possible re-enterant, keying Enter will replace it.

To delete an entire group; when selecting a group to edit do not key Enter following the group number but instead key Del. This will remove the group from the list. If this was the last group then subsequent re-entry to the Edit Group option will automatically go into entering a new group.

4.4.4.5 Store Current Spectrum In Library

If you wish to save your real spectrum as a library entry this can be done using option 4. You will be offered the next blank entry in the library to save your spectra or you can type in your own number to overwrite an existing entry.

The highest peak in the spectrum will be allocated 100%, with the next fourteen highest peaks scaled accordingly. It is this information which, along with the name and formula you label it with, will be stored in the library.

When you have entered this information the data will be stored in the library file.

4.4.4.6 Save Scan In NIST Format

The NIST Standard Reference Database contains approximately 50,000 mass spectra. It is possible to save either a Log or a Linear Histogram Scan in a format which can be read by the NIST package. The 'User Spectra' can be directly compared with the spectra in the database or searched through the database.

When the Save Scan option is selected you will be requested for a filename. This filename is given the suffix **.NBS**.

This **.NBS** file cannot be examined using Quasar but is in the correct format for the NIST library, option U (User Spectra). These **.NBS** files are stored to disk using the same directory path as other Quasar data files.

The NIST library software is available from VG Quadrupoles.

4.4.4.7 Alter Search Parameters

This option allows alteration of the parameters used by the software during the Library Search.

The two parameters are:

Validation Confidence Factor [0-4]

The software will go through each possible list item and remove it from the calculations. If there is not a statistically significant worsening of the fit then the item is deemed not a significant component. A statistical F-Test metric is used to carry out the validation.

The F-Test confidence factors are:

0 No validation is carried out

1 30% confident that the items are present

2 50% confident that the items are present

3 70% confident that the items are present

4 99% confident that the items are present

Further details are given in Appendix E.

Inter-Gain Range Weighting Factor [1.0-10.0]

This factor takes into account the significance of values on higher sensitivity gain ranges. The higher the factor the more credence is given to the higher sensitivity ranges.

A default value of 5.7 assumes that less significance should be given to the higher sensitivity ranges than a value of 10.0.

4.4.5 Live/Review Log Histogram Comparison

The last two options of the HISTOGRAM SCAN menu are concerned with the Log Histogram compare mode of operation. This mode allows you to display a stored log histogram file and a live run on the same screen.

The displayed stored scans can be taken from several log histogram files. The filenames and the relevant scan numbers are stored in an ASCII file called a SEQUENCE file.

4.4.5.1 Creating a Sequence File

The sequence file merely contains a list of those files and scan numbers that will be displayed with the live log histogram run.

Set up the SEQUENCE file as follows:-

1. Select option 5 of the HISTOGRAM MENU. You will then be shown a summary of the set up procedure. Press a key to continue.

SET-UP SEQUENCE PROCEDURE SUMMARY

Here is a summary of the actions you will take

- (a) Choose sequence file name.
- (b) Select log histogram file(s).
- (c) Select scan. Key Ent on SCAN# box to store in sequence file.
- (d) Optional edit of scan numbers and labels.

Strike any key to continue; Esc to cancel

2. If there are no SEQUENCE files in the data directory you will be informed of this. Otherwise you will be presented with a list of current SEQUENCE files. Key **End** to overwrite a file or **Esc** to add a new file.

```

List of files in A:\DATA\*.SEQ
 30.2% free disk space 109568 bytes free

NEWPROC 01 Jan 80 00:09 75 SEQUENCE file
PROCESS1 01 Jan 80 00:06 133 SEQUENCE file

```

3. You will then be presented with a list of log histogram files.

```

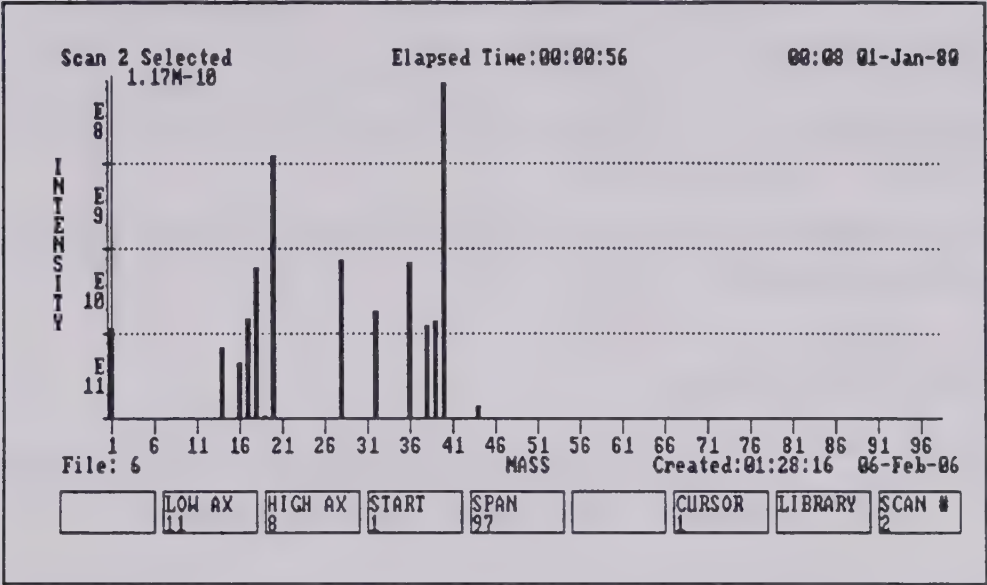
List of files in A:\DATA\*.lgh
31.1% free disk space 112640 bytes free

AH      11 Jul 90 17:26 488 Log Histogram
ASPIRIN 24 Apr 90 14:08 40437 Log Histogram

Sort by 2:Date 3:Group and name 4:Group and date
Key * to select file; Esc to cancel

```

Select a suitable file and review it. Use the cursor keys in the SCAN box to display a suitable scan record. Key Ent to add this record to the SEQUENCE file. A message in the top left hand corner of the screen will confirm your choice. Several scans may be taken from a file.



4.
- Key Esc to return to the list of log histogram files. At this point you may select another file and go through step 3 again. Key Esc again to move to the next step.
5.
- This step is the SEQUENCE EDIT PAGE. At this point you may change the scan numbers and add optional labels. These labels will be displayed at the top of the live/review run screen.

SEQUENCE EDIT PAGE		
FILE	SCAN	LABEL
6.LGH	1	beginrun
6.LGH	2	
6.LGH	5	middlerun
ASPIRIN.LGH	1	
ASPIRIN.LGH	2	
ASPIRIN.LGH		endrun

Enter data in screen format; key * to accept; key Esc to cancel

6. Key **End** to accept the data and create the SEQUENCE FILE. Key **Esc** to cancel the whole operation.

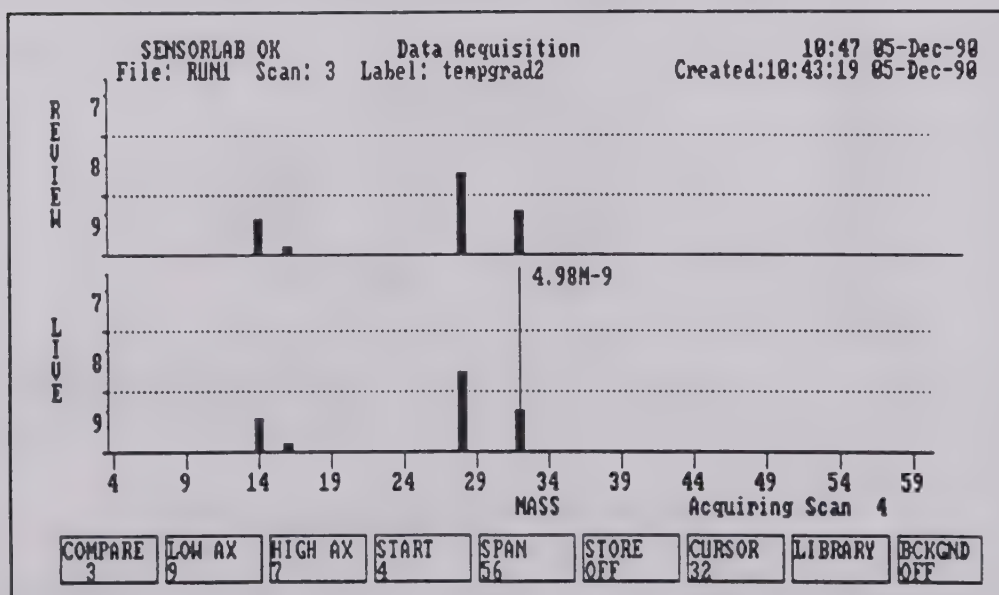
It is important to note that the scans may be selected from one file or several files, and that there is a limit of 10 scans per SEQUENCE file.

4.4.5.2 Live/Review Run

Once a SEQUENCE file has been created you may then proceed to perform a log histogram live/review comparison.

The procedure is as follows:-

1. Select option 4 of the HISTOGRAM MENU. A list of SEQUENCE files in the current data directory will be displayed. Select one file.
2. You will then be presented with the LOG HISTOGRAM PARAMETERS EDIT PAGE. This is the usual edit page that precedes a live log histogram run. Choose suitable parameters and key **End** to accept.
3. A screen similar to the one in the figure will be displayed. The top graph is for review and the bottom is for live.



4. To view the data records mentioned in the sequence file, use the cursor keys in the **COMPARE** box. The appropriate filenames, scan numbers and labels will appear at the top of the screen. Initially, the first entry in the **SEQUENCE** file will be displayed.

Please be aware that the sequence files do not contain individual scan records of data. They only contain filenames, scan numbers and labels. Using this information the software can determine which scan is recorded from a file to load in. Therefore be careful when deleting log histogram files.

4.5 Multiple Ion Monitoring

This mode allows up to 16 mass components to be selected for analysis. A recipe is constructed specifying the mass, detector, accuracy of measurement and other storage/display features for each channel. The recipe can be stored to disk for subsequent use.

The MIM option offers a number of features to aid analysis of gaseous components present in the ion source of the mass spectrometer:

A TREND ANALYSIS

The signal of up to 16 components can be plotted in colour on a logarithmic graph, giving immediate visual indication of any changes within the vacuum system.

B BACKGROUND SUBTRACT

The contribution from background peaks can be subtracted from the peak select data, thus allowing easy analysis of samples subsequently added to the vacuum system.

C RELATIVE SENSITIVITY

Correction factors can be entered for each component to account for the sensitivity of the analyser and efficiency of ionization. This facility can give more accurate results as not all gases are detected with the same sensitivity by the RGA.

The sensitivity of an analyser is quoted in Amps/mb for Nitrogen, ie the relative sensitivity factor for Nitrogen is 1.0. For a more detailed explanation of the factors which affect the sensitivity of a quadrupole analyser to a given gas, refer to Appendix D.

D ALARM LEVELS

High and low alarm levels can be set for any number of components, triggering the display, audible alarm and relay contacts when the alarm level is breached.

E PRINT OF DATA

If a printer interface card is installed, data collected during the run can be printed periodically according to number of cycles or time.

F DATA STORAGE

Some or all of the peak select can be stored to disk for subsequent analysis. Data file names are user defined.

G TIMED CYCLING

The peak select program can be set to free run, by entering a value of zero, and cycle through the measurements as quickly as they are recorded. Alternatively, the time interval between measurement cycles can be set from 100ms to 1 hour

On selecting option 4 from the Main Menu, Multiple Ion Monitoring, a sub-menu appears:



Data Acquisition

MULTIPLE ION MONITORING

[1] Edit Recipe

[2] Run

[3] Acquire Backgrounds

[4] Clear Backgrounds

[5] Alarms ON/OFF

[6] Recall Stored Recipe

Please key option

Quasar Software

6.5.1 Edit Recipe

Selecting option 1 from the MIM Menu leads to the Edit Recipe screen:

RECIPE NAME: Default

NO CYCLES [0 - 65535]: 100

CYCLE-PERIOD IN 1/10 SEC [0 - 36000]: 10

STORE RECIPE [No/Yes]: No 0:No

PRE PEAK-LOCK [No/Yes]: Yes 1:Yes

PRE ZEROING [No/Yes]: No

CHANNEL	ENABLED	DETECTOR	MASS	NAME	ACCURACY	RANGING	RANGE	REL/SENS	STORE
1	No	Faraday	2	Hydrogen	2: 16	Constant	7	1.000	No
2	No	Faraday	4	Helium	2: 16	Constant	7	1.000	No
3	Yes	Faraday	18	Water	2: 16	Auto	7	1.000	No
4	Yes	Faraday	28	Nitrogen	2: 16	Auto	7	1.000	No
5	Yes	Faraday	32	Oxygen	2: 16	Auto	7	1.000	No
6	Yes	Faraday	40	Argon	2: 16	■	7	1.000	No
7	No	Faraday	44	CO2	2: 16	Constant	7	1.000	No
8	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
9	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
10	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
11	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
12	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
13	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
14	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
15	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No
16	No	Faraday	28	Nitrogen	2: 16	Constant	7	1.000	No

0:No 0:Faraday

1:Yes 1:SEM

Accuracy 0:Constant

1 2 3 4 1:Auto

0:No

1:Yes

Enter data in screen format; key * to accept; key Esc to cancel

The screen is divided into a number of 'fields'. The highlight can be moved from one field to the next by pressing the **Ent** key. To move quickly to the field to be edited, the ← and → keys can be used to change rows, and the ↑ and ↓ keys to change column position.

There are 5 parameters at the top of the screen to define and control the 16 channel recipe. The heading parameters are defined as follows:

1 RECIPE NAME:

This field shows the name assigned to the recipe. The name can be changed if the recipe is to be edited and stored to disk. The recipe name can be up to 8 alphanumeric characters (do not use spaces or punctuation marks).

2 STORE RECIPE [Yes/No]:

This field determines whether the recipe is stored to disk or not.

If the recipe name is chosen to be called **DEFAULT** and the recipe is to be stored to disk, then this recipe is loaded on power on.

Thus, if a user wishes to monitor only certain masses under certain conditions from day to day it is wise to store the recipe as **DEFAULT**.

3 NO CYCLES [0-65535]:

The number in this field determines how long the peak select program runs before automatically stopping. An entry of **0** means the program runs forever, or until **Esc** is pressed. An entry of **1000** causes the run to stop after 1000 cycles of peak select data have been collected.

4 PRE-PEAK LOCK [Yes/No]:

The location of the mass peak top of each enabled channel can be searched and locked into memory by executing a Peak Lock routine. Select **Yes** for Pre-Peak Lock.

See later section for further details on peak locking.

5 CYCLE-PERIOD IN 1/10 SEC [0-36000]:

The time interval between cycles can be set in this field, enabling a constant data collection rate no matter what the level of signal. The interval can be set in the range 0 to 36000 1/10ths second (ie 100ms to 1 hour).

An entry of **0** sets the Run cycle to free-running, with no added software delays.

If the specified interval time is set less than the time it takes to complete a measurement, then the program behaves as though it were free-running, except that account is taken of the actual time of measurement when the data is plotted.

The main body of the recipe displays ten column headings which apply to each of the peak select channels:

1 CHANNEL

This column cannot be changed, it displays the pre-set channel reference number.

2 ENABLED

An entry of either **Yes** or **No** is allowed, which defines whether the channel is enabled or disabled from the measurement cycle.

Enable only those channels required, since enabling extra channels slows down the cycle time.

3 DETECTOR

This field defines the detector type, either **Faraday** for the Faraday detector or **SEM** for the multiplier, by pressing **F** or **S** respectively. Entering a value of **U** sets that channel to read one of the two user analogue inputs. Refer to section 6.5.1.1 for details of analogue inputs.

If the multiplier is not switched on, the user will be informed that the multiplier is off. The **SETUP MASS SPEC** page will then be entered.

4 **MASS**

Enter the mass number (integer only) of the species to be measured on this channel. Type new mass number over existing value, ensure that no digits from previous value remain. If in the detector column you have selected '2' for user analog inputs, then in the mass column you enter 1 or 2, depending on which analogue input you wish to monitor.

An entry of 0 programs a total pressure measurement.

5 **NAME**

This field allows the user to enter a recognisable name against a particular channel thus allowing easy identification of the mass species.

Up to 9 characters can be entered by using the text insert mode by pressing the ? key. Key Esc to leave the text editor.

6 **ACCURACY**

This field relates to the accuracy of the measurement.

- 1 Single measurement regardless of gain range. Fastest measurement type.
- 2 Normally the average of 16 readings, but this is increased for some gain ranges. Designed to provide same signal to noise performance on each gain range. Ideal general purpose accuracy code.
- 3 The average of 16 code-2 readings.
- 4 The average of 256 code-2 readings.

7 **RANGING**

This field can either contain *AUTO* or *CONSTANT*. Auto indicates that the analysis is automatically autoranging, ie under software control the amplifier is switched to the gain range most suited to the signal level. A *CONSTANT* entry indicates that the amplifier gain is fixed according to the range defined in column 8.

8 RANGE

This field defines the gain range used in the *CONSTANT* mode, or the initial gain setting in Autoranging mode.

Entries from 5 to 10 are allowed for the Faraday detector, and from 7 to 13 for the SEM.

9 REL/SENS.

A relative sensitivity factor from 0.01 to 99.99 is entered in this field. The measured signal is then divided by this factor to produce the corrected data which is displayed on the screen during RUN.

10 STORE

Some or all of the measurement cycle data can be stored to disk. This column programs whether the channel requires data storage (**Yes**) or screen only logging (**No**). If one or more channels are enabled for data storage, then a data file name is requested at the commencement of a run.

When all the functions described above are programmed and the recipe is complete, key **End**. The whole screen is then processed.

The software processes the whole screen and produces an error message if any of the field entries are invalid, if an error is found the highlighted pointer automatically steps to the field in error and awaits the entry of a new value. The screen clears to recipe storage prompts if the Store Recipe option has been selected.

The recipe name can be changed at this stage. Press **End** when the desired name is shown to initiate the storage to disk.

The screen now returns to the *MULTIPLE ION MONITORING* (MIM) menu.

4.5.1.1 User Analogue Inputs

In multiple ion monitoring mode it is also possible to monitor external analog inputs via pins 17 and 18 of the SKT2 socket, see section 7.3.1. The analogue inputs are required to be in the range -10V to +10V and can come from virtually any calibrated measuring instrument.

As an example, you may wish to monitor several masses over a period of time but also keep track of the temperature. A suitable temperature measuring device that provides an output voltage corresponding to a temperature is required.

PROCEDURE

1. Select option 1 of the Multiplie Ion Monitoring menu. Edit the recipe. Up to 2 channels (or 16 channels if you have a DT2814 interface card) may be selected for user analogue inputs.
2. To select a channel for a user input instead of a specific mass move the highlighted cursor to the **DETECTOR** column of the selected channel. Type 'U' and the word **user** will appear.
3. To select one of the analog inputs move the highlighted cursor to the **MASS** column. Type in '1' or '2' (or '1' to '16' for DT2814 interface) for the analog input number.
4. When the recipe has been processed you will be presented with the Analogue Inputs edit page, see diagram. At this point you can name the user inputs, e.g. Temperature. You will also be requested for the scaling, e.g. 0V to 10V may represent 10°C to 60°C. Key **End** to accept the data.

ANALOGUE INPUTS: NAME AND SCALING	
Axis label name:	Temperature
Mode: choose scale...	Positive
Positive: 0v to +10v	
Bipolar: -10v to +10v	
+10v corresponds to:	100.00
0v corresponds to:	
-10v corresponds to:	-100.00
Enter data in screen format; key End to accept; key Esc to cancel	

5. Select option 2 of the Multiple Ion Monitoring menu to run.

In table mode the analogue input name is in the **ACCURACY** column and the input number is in the **MASS** column. The reading will be in user specified units, not volts.

In trend mode a linear user axis will be displayed on the right hand side of the trend graph by keying **Ent** in the **USER** box.

The standard SENSORLAB is limited to only 2 analog inputs but this can be oincreased by up to 16 by fitting your PC with a DT2814 interface card. Available from VG Quadrupoles.

4.5.2 Run

Option 2 of the MIM menu is the main *RUN* routine, in which the instrument cycles through the measurements defined by the recipe.

If data storage has been requested for any of the channels, a prompt for a data filename is displayed before any further action is taken.

When the data file is created (if specified) the screen displays only the enabled channels and a flashing message at the bottom of the screen saying **please wait - to abort key Esc**. During this period the optimum gain is selected for each autoranging channel and the peak centers are locked (if Pre-Peak Lock is Yes). When a peak centre is found the exact mass position according to the computers scaling is displayed in between the channel number and the mass.

At the end of this initialisation routine the SENSORLAB software prompts:

key End to start run

The instrument is ready and waiting for the signal to start the run. Key Esc to cancel.

4.5.2.1 Table Mode

The signal measurement is shown against each enabled channel, with the letter before the exponent indicating the detector type used for the measurement.

The cycle number and elapsed time since the *RUN* started are shown below the enabled channels.

RECIPE NAME:Default			Data Acquisition			00:02 01-Jan-80	
CHANNEL	MASS	NAME	ACCURACY	GAIN	REL/SENS.	READING	
3	18	Water	2	F 7	1.000	2.16F-7	
4	28	Nitrogen	2	F 7	1.000	1.96F-7	
5	32	Oxygen	2	F 7	1.000	1.69F-7	
6	40	Argon	2	F 7	1.000	1.67F-7	
							TIME:00:00:17
DISPLAY TABLE	PRNTCYC 0	PERCENT OFF			STORECYC 0		CYCLE # 15

At the bottom of the screen there are 9 option boxes. These options can be accessed and changed before starting the run.

BOX 1 DISPLAY

Selecting this option switches the display mode to Trend.

BOX 2 PRNTCYC

This option applies only if a printer is connected to the your PC. Tabular data can be sent to the printer by entering a number to define the frequency of output. For example, using the ↑ key until the number in the box is 10, followed by **Ent** causes every 10th cycle of data to bedumped to the printer. Entering 0 stops the printer output.

BOX 3 PERCENT

Pressing **Ent** causes the measurements except total pressure to be expressed in percentage format. **ON** is displayed in the box. 100% corresponds to the sum of all the partial pressures of the enabled channels.

Press **Ent** again to revert to partial pressure display format, the box then shows **OFF**.

If extremely fast data collection is required then we recommend you maintain the partial pressure display.

BOX 4 Not used in Table mode

BOX 5 Not used in Table mode

BOX 6 STORECYC

This option defines the frequency of data storage to disk. The default values are **0** (no storage) or **1** if data storage is programmed in the recipe.

An entry value of **1** means that every measurement cycle is stored, while an entry value for **10** programs every 10th cycle to be recorded. The STORECYC frequency can be changed during the Run. Press **Ent** after updating the number using the **↑** or **↓** keys to effect the change.

BOX 7 Not used in Table mode

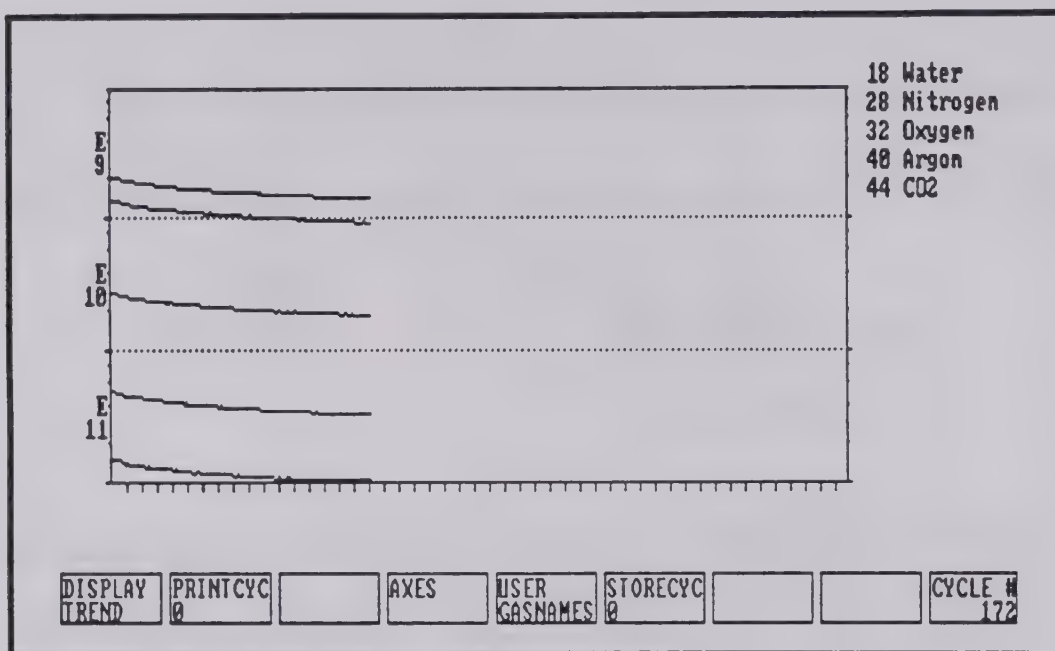
BOX 8 Not used in table mode

BOX 9 CYCLE #

This box displays a running count of how many measurement cycles have been taken since the start of the run.

4.5.2.2 Trend

This display mode is accessed from the MIM RUN option and gives a logarithmic graphical representation of the output of all enabled channels:



The masses and names of the selected channels are shown in up to 16 separate colours beside the graph. Lines of corresponding colours map the pressure changes for that compound.

The dynamic range covered and the detector type are depicted along the y-axis. The x-axis is scaled and labelled as a linear elapsed time axis if a timed cycle has been specified, otherwise the cycle number is displayed.

If the printer option is fitted, a dump of the screen image can be made at any time by pressing the **Prt** key.

At the bottom of the screen are 6 active option boxes similar to the Tabular display.

BOX 1 DISPLAY

Selecting this option by pressing **Ent** reverts the screen display to the Tabular mode.

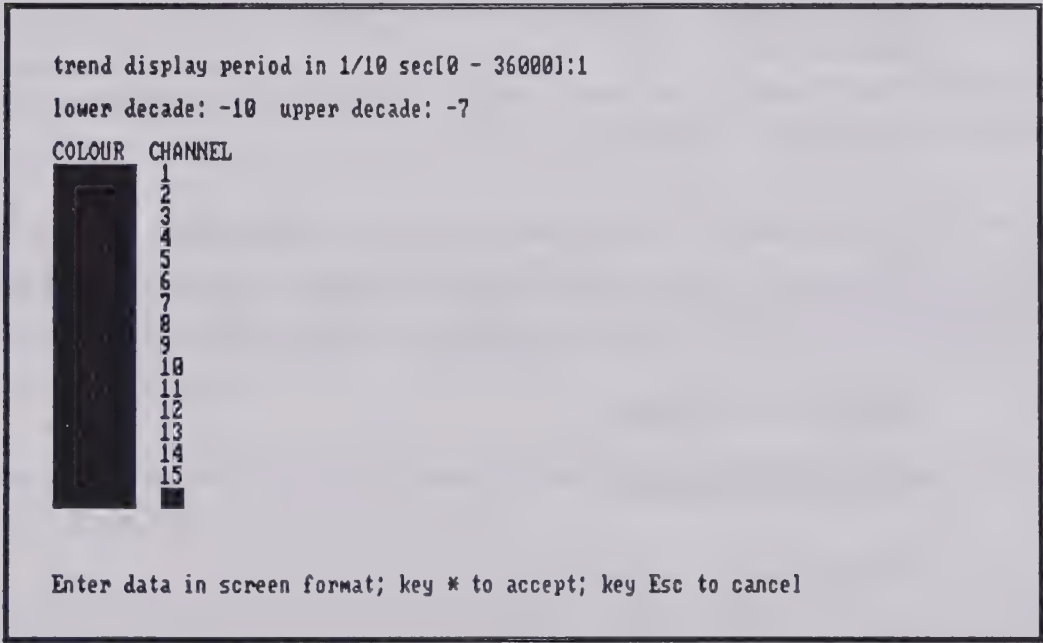
BOX 2 PRINTCYC

This option applies only if a printer is connected to the your PC. Tabular data can be sent to the printer by entering a number to define the frequency of output. For example, using cursor up until a value of **10** is reached followed by **Ent** causes every 10th cycle of data to be dumped to the printer. Entering **0** stops the printer output.

BOX 3 Not used in Trend mode

BOX 4 AXES

This option leads to a screen editor menu which defines the display parameters.



The entry highlight can be moved through the parameter options with the **Ent** key. The **↑** and **↓** keys allow quick movement between rows.

The top line defines the time interval used for plotting the data. This value defaults to the same as set in the recipe. The plotting time interval can be changed whilst retaining the data acquisition rate previously defined. If a value of zero is stored then each data point is plotted as one horizontal pixel.

The second line defines the y-axis parameters. The number of decades can be set by defining the lower and upper decades to be displayed. The limits are -5 (upper) to -15 (lower).

The pressure axis is normally displayed in a quasi log format, however, if you select an axis with a single decade (ie upper gain = lower gain) then the pressure axis will be in a linear format.

When editing of the display format is complete key **End** to return to the re-defined trend display screen.

BOX 5 USER GAS NAMES

Press **Ent** to toggle between gas names and axis for analog inputs (if enabled).

BOX 6 STORECYC

This option defines the frequency of data storage to disk. The default values are **0** (no storage) or **1** if data storage is programmed in the recipe.

An entry value of **1** means that every measurement cycle is stored, while an entry value for **10** programs every 10th cycle to be recorded. The STORECYC frequency can be changed during the Run. Press **Ent** after updating the number using the **↑** or **↓** keys to effect the change.

BOX 7 Not used in Trend mode

BOX 8 Not used in Trend mode

BOX 9 CYCLE #

4.5.3 Acquire Backgrounds

This mode resembles a *RUN* screen except that data is collected to record the average background measurements at each enabled mass. If the *CYCLES* entry in the Recipe is zero, the background values are taken as the average of 16 measurement cycles. If the *CYCLES* value is non-zero, that many measurement cycles are averaged.

The letters **BG** are shown on the screen to indicate that background measurements are being recorded. During data acquisition a running average is displayed; press **Esc** to return to the Menu after the display stops updating. Subsequently all data is corrected by subtracting this background data from the measurements recorded during a run.

4.5.4 Clear Backgrounds

Selecting this option clears the background values from memory and thus 'switches off' Background Subtraction.

4.5.5 Alarms

The alarm facility is only available in the MIM mode of operation and allows the user to set pressure limits (both partial and total) which when breached alter the state of relay outputs for HIGH and LOW levels.

The facility is toggled ON/OFF by repeated presses of '5' in the MIM sub-menu. The current state either ON/OFF is shown in yellow text.

When you complete the edit recipe page, if the Alarm facility is enabled then the next page displayed is the "Edit Alarms" page. You are first asked to specify if the units for alarm levels are to be in partial pressure or percentages, and press **End** to confirm your choice.

The actual alarm edit page, shows the channel you have enabled and allows you to set values within the limits of the detector you have selected.

When in the RUN mode of MIM, the alarm levels you have set will be compared to the pressure/percentage readings being measured, and if any limit is breached then the words LOW and HIGH will be displayed in the ALARM column, and the corresponds relay will change state accordingly.

To prevent relay "chatter" there is a built-in hysteresis of 10% of signal value when alarm levels are crossed.

4.5.5.1 TTL Alarm Outputs

If you have ordered a DT2817 interface card with your SENSORLAB then the HIGH and LOW alarm signals will appear as TTL voltage outputs (0V or 5V) from this card.

The DT2817 has four 8 bit input/output ports for digital TTL signals. The connector is a 50 way 3M type. Only 32 of the 50 available lines are used for data.

The SENSORLAB software configures all four ports for output only. Each of the 16 MIM channels is assigned 2 pinouts. One pin for the LOW alarm signal and one for the HIGH signal.

If both pinouts for a particular channel are logical 0 (0 volts) then the measured signal for that channel is within the specified limits. If one pinout is logical 1 (5 volts) then either the HIGH or LOW alarm has been triggered. Note that both pinouts cannot be logical 1 at the same time.

This can be summarised as follows:-

LOW	HIGH	MEANING
0	0	Signal is within limits
0	1	Signal above upper limit
1	0	Signal below lower limit
1	1	Not allowed

The outputs of the four data ports are arranged as follows:-

PORT	MIM CHANNELS	ALARM STATE
0	1 - 8	LOW
1	1 - 8	HIGH
2	9 - 16	LOW
3	9 - 16	HIGH

For details of the port pinouts see the DT2817 user manual, table 4-2, page 4-4.

The base address of the DT2817 is set to 2F0 and must not be changed.

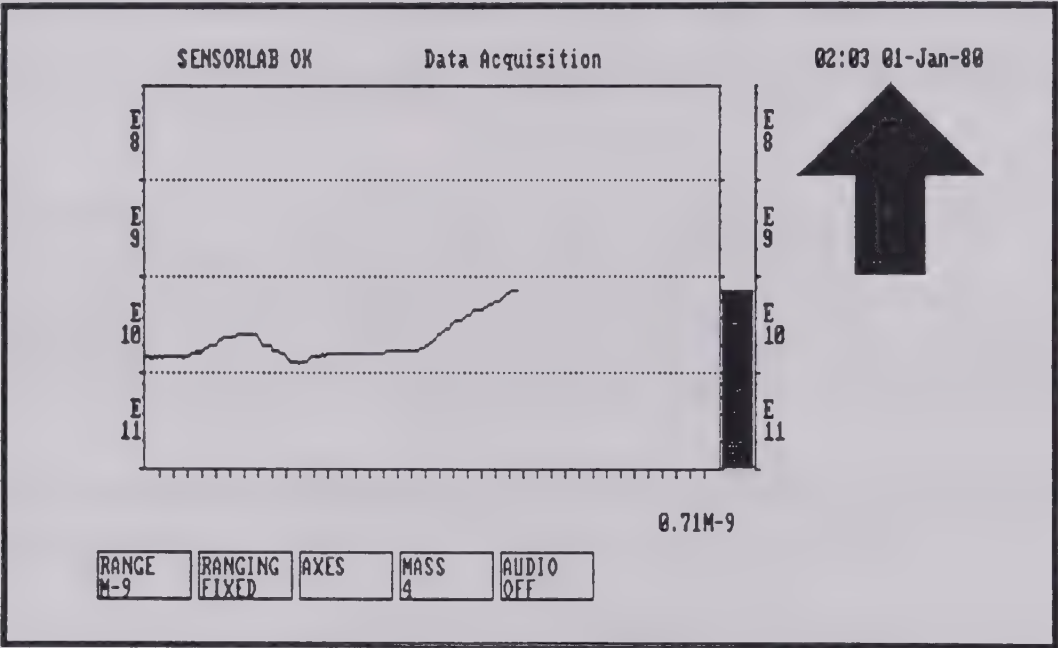
4.5.6 Recall Stored Recipe

This option allows a recipe stored on disk to be read into memory. The user will be presented with a list of recipe files held on the default disk drive. Use the ↑ and ↓ arrows to move the highlighted bar to the desired filename. Key **End** to load in the recipe.

This recipe may then be viewed and edited by selecting option 1 of the MIM menu.

4.6 Leak Detection

Leak detection mode allows the user to isolate the source of a leak and minimise down-time of the system. The mode is controlled by the parameters in the function boxes. The partial pressure of the gas in the system is shown graphically as a column, with a corresponding digital read-out on the right hand side. If the screen cannot be seen, use the loud speaker output. If totally remote from the instrument then an analogue output is available via the chart recorder output for feeding to a DVM.



BOX 1 RANGE

Use the ↑ and ↓ keys to alter the gain accordingly. Change will appear in the box while the range is being changed.

BOX 2 RANGING

Use the **Ent** key to toggle between FIXED and AUTO gain range.

BOX 3 AXES

This page allows the user to set which gain range or ranges are displayed.

For a fine leak you would set a single decade axis to see small variations. For a gross leak use a three or four decade plot depending on the size of leak.

Press **End** to implement the changes.

BOX 4 MASS

The default MASS is 4 (for Helium), but this can be changed to any other desired mass (within the range of the instrument) by using the $\uparrow$ and $\downarrow$ keys and pressing **Ent** to confirm.

BOX 5 AUDIO

An audible leak signal is provided via the loud speaker on the instrument. Use the **Ent** key to switch this *OFF* or *ON*.

The display shows a yellow box for a static pressure reading, if the signal intensity rises indicating more trace gas entering the system a bold up arrow is displayed in red, if the leak is cured and the trace gas is pumping away (a good condition) then a bold green down arrow is displayed as long as the pressure trend is continued. The partial pressure for the mass selected is plotted against time, over the pressure range(s) selected.

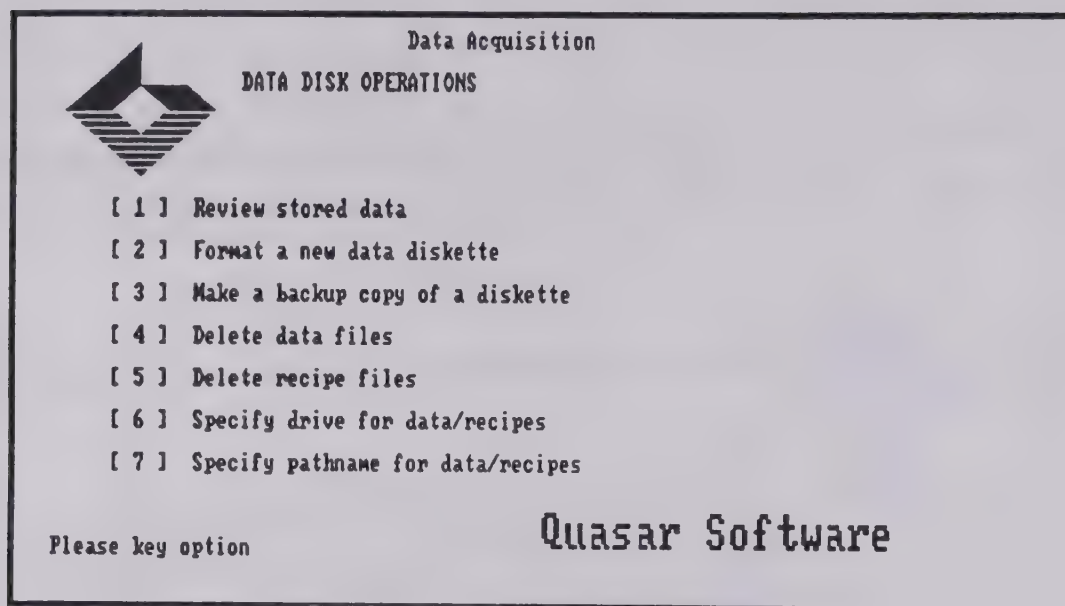
This leak detection mode can equally be used as a Single Ion Monitor.

The pressure intensity signal is also provided via the chart recorder output (SKT2) as a voltage from 0 to 10 V for the decade in which the reading is taken. For example a reading of 5.3×10^{-7} would appear as 5.3 V.

Pressing **Esc** leaves Leak Detect mode, and returns to the main menu.

4.7 Data Disk Management

Options are selected from a sub-menu:



4.7.1 Review Stored Data

Selecting option 6 from the Main Menu leads to the data retrieval and display program. This allows data collected to be reviewed.

A directory of data files is displayed from the default data drive. Using the ↑ and ↓ keys move the highlighted bar over the filename you wish to review. Key **End** to review this file. Key **Esc** to return to the **DATA DISK OPERATIONS** menu.

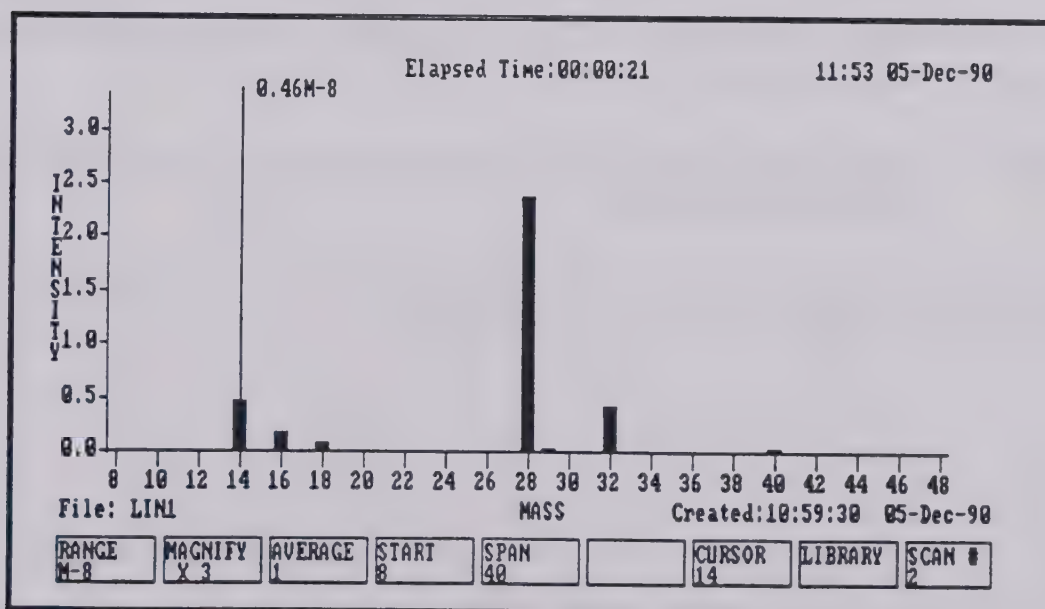
The program automatically determines the data type (which type of scan mode) and displays the appropriate screen. To advance through the data, go to the function box marked 'SCAN #', and press the ↑ key. To go backwards, use the ↓ key.

List of files in A:\DATA*. *
38.1% free disk space 138240 bytes free

1	05 Apr 90	14:24	3679	MIM data
22	05 Apr 90	14:40	871	MIM data
3	01 Jan 80	03:11	9158	MIM data
3333	05 Apr 90	14:49	1703	MIM data
5	01 Jan 80	02:08	13366	MIM data
56	14 Jun 90	13:39	1315	Linear Histogram
6	01 Jan 80	00:49	31299	Log Histogram
AH	11 Jul 90	17:26	488	Log Histogram
ANTEST1	03 May 90	13:47	3715	Analogue
ANTEST2	03 May 90	13:55	4937	Analogue
ASPIRIN	24 Apr 90	14:08	40437	Log Histogram
CUSO4	15 Feb 89	10:39	65520	MIM data
HIST1	03 May 90	13:49	481	Linear Histogram
M1	05 Apr 90	14:29	1183	MIM data
POLY1	16 Feb 89	12:48	9414	MIM data
POYL2	16 Feb 89	16:06	7318	MIM data
XEAIR	11 Nov 88	12:35	1271	Analogue

Sort by 2:Date 3:Group and name 4:Group and date
Key End to select file; Esc to cancel

Histogram and Analogue data review is operated in a similar manner to the real time mode.



The function boxes available to control the data are;

- | | | |
|---|---------|---|
| 1 | RANGE | - not accessible, only shown for reference. |
| 2 | MAGNIFY | |
| 3 | AVERAGE | - not accessible, only shown for reference. |
| 4 | START | - not accessible to analogue scan data. |
| 5 | SPAN | - not accessible to analogue scan data. |
| 6 | STORE | - not accessible, only shown for reference. |
| 7 | CURSOR | |
| 8 | LIBRARY | |
| 9 | SCAN # | |

Likewise MIM data review is almost the same as a real time run.

Press **Esc** to return to DATA DISK OPERATIONS MENU

4.7.2 Format A New Data Disk

To be able to store spectra on a blank disk, it first must be prepared to accept data, this operation is called disk formatting. The type of blank disk(s) you require are "double sided, double density, 48 TPI" for a 5¼ " unit, and 720K for 3 ½" drives.

CAUTION: If re-cycling an existing disk, any information already on disk will be deleted, and cannot be recovered.

The formatting operation checks the disk media surface is free from defects and writes a structure to the disk allowing storage of both DATA and RECIPE files.

After the first disk is formatted, cancel the operation by pressing the N key, following the instruction on the screen.

CAUTION:

Be warned that in order to perform formatting and disk copying the SENSORLAB software exits its program and therefore all data acquisition processes will be terminated.

If you do not have a hard disk installed in your PC then you may be prompted to insert the START UP DISK. This is necessary in order to load into memory the appropriate utility i.e. the DOS format or disk copy program.

At the end of the format or disk copy routine you may be asked to insert the SYSTEM DISK. This is necessary in order to re-load the SENSORLAB program.

If your PC has a 3½" disk drive then the START UP and SYSTEM disks are one and the same. If you have a 5¼" drive then the START UP and SYSTEM disks are two separate disks.

4.7.3 Making A Copy Of A Diskette

To protect the master or "source" disk against accidental erasure on a 5¼", place a "write-protect" sticker over the small notch on the edge of the disk jacket (not over the disk surface) and on a 3 ½" disk slide the black insert in the case.

The user is then prompted on the screen to insert your "SOURCE" disk and blank "DESTINATION" disk alternately.

Press the 0 key to cancel the operation when prompted on the screen.

See the second cautionary note in 6.7.2.

4.7.4 Deleting Data Files

By using the ↑ and ↓ keys it is possible to select any file for deletion. This can be any file in the displayed directory. Key Del to delete a file. You will then be prompted to key Ent to confirm the deletion.

```
List of files in A:\DATA\*.*
8.6% free disk space 61952 bytes free

ANAL1  05 Dec 90 11:00 2493 Analogue
LIN1   05 Dec 90 10:59 593  Linear Histogram
PROCESS1 05 Dec 90 10:46 93  SEQUENCE file
RUN2   05 Dec 90 10:45 1927 Log Histogram

Sort by 2:Date 3:Group and name 4:Group and date
Key Del to delete file; Esc to cancel
```

4.7.5 Deleting Recipe/Profile Files

This is identical in operation to the procedure for deleting a data file

4.7.6 Specify Drive for Data/Recipes

This facility enables data and recipe files to be accessed on any of the available disk drives.

Key in the number corresponding to the drive you wish to select and **End** to accept.

Change default drive for data to:

1. A:
2. B:
3. C: ← Current default
4. D:
5. E:

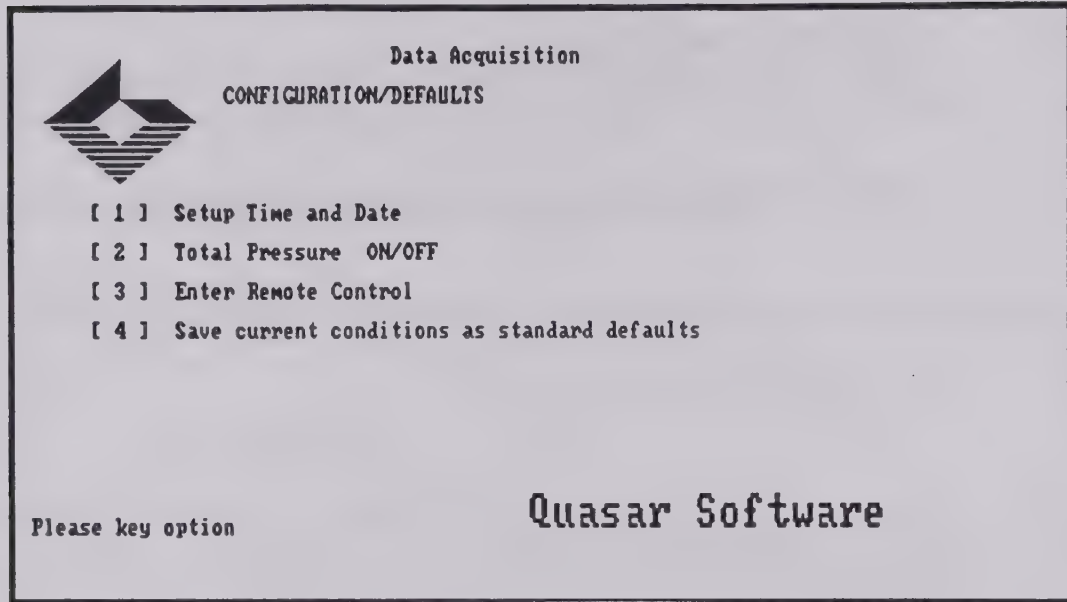
Key drive letter or number; key End to accept; Esc to cancel

It should be noted that systems executing from floppy disk will only have options for drive A: and B:.

It should also be noted that systems with a single floppy disk drive reference this drive as both A: and B:. The one physical disk drive is divided into two logical drives with prompts from the system telling you to insert a disk for drive A and B.

4.8 Configuration/Defaults

This option allows some of the system parameters to be set up.



4.8.1 Setting Time and Date

This option allows the system time and date to be set.

In order to perform this option the system temporarily exits to DOS in order to load in the clock setup program. As with formatting and disk copying (section 4.7.2) you may be prompted to insert the START UP DISK in order to load in the time setting program. When the routine has finished you will be prompted for the SYSTEM DISK in order to reload the system.

4.8.2 Total Pressure

When set to ON this option enables a total pressure measurement prior to each Analogue and Linear Histogram scan. The total pressure is displayed below the mass axis on the right hand side. Key '2' to toggle between ON and OFF.

4.8.3 Enter Remote Control

Selecting this option initiates remote control.

The remote control option relies on a special ASCII communications protocol. This allows one to remotely set scan parameters and receive data from virtually any host via a serial link.

Remote control is described in detail in Appendix F.

4.8.4 Save Current Conditions

When Quasar is loaded into memory it is possible for it to come up in a pre-defined state.

Selecting option 4 will save the current system parameters in a disk file. The systems parameters include emission state, SEM volts, gain ranges and mass ranges for scans etc. Exiting to DOS via the Main Menu will also cause the system parameters to be saved.

NOTE: If your PC does not have a hard disk please place the **SYSTEM DISK** in the drive before selecting this option. The system parameters will then be written to the **SYSTEM DISK**, and therefore can be re-loaded when the instrument is switched on again.

4.9 Dual Tasking

One of the major features of Quasar software is the ability to acquire data and review stored data at the same time. This is made possible by special dual tasking software and the fact that the EGA graphics adaptor can store up to 4 screen of information.

The two processes or screens have titles "Data Acquisition" and "Data Review". The first process has access to all data acquisition and data review facilities. The second process is limited to data review only.

4.9.1 Screen Switching

To switch between processes use the <SHIFT>F1 and the <SHIFT>F2 keys in the following manner.

While running an analog scan, for example, press <SHIFT>F2 You will then be presented with the **DATA DISK OPERATIONS** menu. At the top of this menu page will be written "DATA REVIEW" to signify that you are in the second process. you now have access to all the functions associated with this menu while process one is still running. To switch back to process one, press <SHIFT>F1.

To summarise:-

<SHIFT> F1 - Process 2 to process 1

<SHIFT> F2 - Process 1 to process 2

Process 1 - Data Acquisition

Process 2 - Data Review

4.9.2 Example Uses of Dual Tasking

- a) Comparing today's live scans with yesterday's stored scans.
- b) Comparing two separate stored files.
- c) Comparing two different scans from the same file.

The latter two are made possible by the fact that both processes have a **DATA DISK OPERATION** menu.

4.9.3 Format and Disk Copy on Screen Two

It is very important to note that the format and disk copy routines exit to DOS before executing. thus if you perform a format or disk copy on screen two, then any task running on screen one will be shut down completely. It is safer to perform these routines from screen one.

5. INSTRUMENT FUNCTIONS

5.1. Principles Of Operation

The Sensorlab system includes an analyser which will measure total pressure and partial pressure. The ranges of operation will depend on the model you have purchased. The analyser can be operated up to 10^{-3} mbar, but prolonged use at these high pressures is not recommended.

The analyser is a quadrupole mass spectrometer, which is capable of separating the ions formed in an electron impact source according to their mass-to-charge ratio. The power to the analyser may also be arranged so that the whole ion beam is transmitted, thereby producing a collected ion current approximately proportional to the total pressure. The signal collector can be of the Faraday cup or SEM type. It is recommended that electron multipliers are not operated at pressures in excess of 10^{-6} mbar.

A general explanation of the operation of the instrument is given in Appendix C.

5.2. Front Panel Controls

There are no user adjustable controls for the Sensorlab unit, the operation of the mass spectrometer is fully controlled by the PC computer. Sensorlab has a front panel switch for Mains Supply

The mains switch is of the double pole type and thus switches both nominally live & neutral supply lines. The front panel led is illuminated from a 15 V DC supply generated when the unit is switched on.

5.2.1 Optional Controls

On certain units depending on the configuration, there may be front panel controls for parameters such as Ion Energy, Focus etc. This will be suitably labelled and have further instructions in a supplementary note.

5.3. Rear Panel

5.3.1 Analogue Input/Output Connections

SKT4 is a 25-way, D type socket for the analogue input/output option (if fitted).

The pin-out for this connector is:

1	Digital Output 1
2	Digital Input 1
3	Digital Output 3
4	Analogue output channel 3 (8 bit)
5	Analogue output channel 4 (8 bit)
6	Analogue Input Ground
7	Analogue output channel 1 (12 bit)
8	Analogue output channel 6 (8 bit)
9	Analogue output channel 9 (8 bit)
10	Analogue output channel 10 (8 bit)
11	DAC 0 V
12	-15 V
13	0 V (P)
14	Digital Input 2
15	Digital Output 2
16	0 V (Digital)
17	Analogue Input 2
18	Analogue Input 1
19	Analogue output channel 2 (12 bit)
20	Analogue output channel 5 (8 bit)
21	Analogue output channel 8 (8 bit)
22	Analogue output channel 7 (8 bit)
23	DAC 0 V
24	DAC 0 V
25	+15 V

5.3.2 MP8X Multiplexer Control

SKT3 is to control a VG MP8X (if option is fitted)

5.3.3 Valve Driver

PL 3 is used only with the Valve driver option.

5.3.4 Auxiliary Input/Outputs

SKT2 provides signals for driving the chart recorder, and for feeding a 'vacuum good' signal to the controller. The pin-out of this connector is as follows;

Pin	Function
1	Scope Y
2	Ramp voltage (X)
3	Chart signal (Y)
4	0 V
6	0 V
8	+5 V, Max current 100 mA
9	Vacuum Interlock

Vacuum interlock is a TTL input normally left floating, but if this line is pulled down to ground potential, it triggers a vacuum failure signal to the Sensorlab, and trips the emission circuit.

5.3.5 Alarms

PL 2 is the plug, providing two sets of relay contacts for high (Relay 2) and low (Relay 1) alarms. The conditions under which these relays are active depend on user settings in the MIM mode. These levels can be set on partial pressure, percentage modes and user values for analog inputs.

RL1	1 - COMMON
	3 - NO (Normally open)
	5 - NC (Normally closed)
RL2	2 - COMMON
	4 - NO
	6 - NC

5.3.8 Voltage

There is an internal PCB capable of re-tapping the instrument to any one of four common voltages. This board must only be removed with the power lead removed. The board is secured by a cable tie, and a new cable tie must be used to secure the board after any changes.

5.3.9 Power Input

The power input (PL1) is a three pin IEC recessed plug. A mating mains lead is supplied with the Sensorlab and requires a suitable plug for the mains outlet.

Observe the colour coding:

ERD KLEMME	GRUN/GLEB
EARTH	GREEN/YELLOW
TERRE	VERT/JAUNE
STROMF UHRED	BRAUN
LIVE	BROWN
SOUS TENSION	BRUN
NEUTRAL	BLAU
NEUTRAL	BLUE
NEUTRE	BLEU

For the USA;

EARTH	GREEN
LIVE	BLACK
NEUTRAL	WHITE

5.3.10 Fuses

The Sensorlab has one externally accessible 3 A anti-surge fuse in the live line, fitted to the rear panel.

A number of other fuses are used on the internal power supplies card as follows;

FS1	1.6 A anti-surge	FS2	100 mA anti-surge
FS3	1.6 A anti-surge	FS4	250 mA anti-surge

**WARNING: FUSES MUST ONLY BE REMOVED OR REPLACED WITH THE
POWER LEAD REMOVED.**

6. OUTPUT OPTIONS

6.1. Parallel printer (other than Epson FX-80 compatible)

The connector on the rear of the computer for a parallel printer is a 25 way D-type plug. The cable to be used is an IBM style cable, or one with connections as shown below;

Computer		Printer
25 Way Connector		36 Way Connector
1	BROWN	1
2	RED	2
3	ORANGE	3
4	YELLOW	4
5	GREEN	5
6	BLUE	6
7	VIOLET	7
8	SLATE	8
9	WHITE	9
10	BLACK	10
11	PINK	11
12	RED/BROWN	12
13	WHITE/BLUE	13
14	NC	
15	YELLOW/RED	32
16	WHITE/RED	31
19	SCREEN	19
20	NC	
21	NC	
22	NC	
23	NC	
24	NC	
25	NC	

NC - NO CONNECTION

To generate a printout of any page press the **Prt Scn** key once.

Ensure that the printer is set to "on-line" before attempting to obtain a hard copy.

6.1.1 Technical Details for Printer

When the **Prt** key is pressed, the screen display freezes and a raster type scan is made of the screen. The pixel pattern is then sent to the printer to form a duplicate image, whilst this is taking place the mass spectrometer operation is suspended.

The default printer support software is for an Epson FX-80 compatible. Other printer drivers are available as an option, from a range of 150 different types (including colour printers).

6.2. Serial Printer

The connector on the rear of an XT type computer for a serial printer is a 25 way D-type socket, and a 9 way-D type on an AT type computer, refer to your computer manual as necessary.

6.3 Analogue Outputs

This option works only in the RUN mode of MIM. For the first ten channels, a voltage (0 to 10V) is fed out through SKT2, ANALOGUE I/O proportional to the reading within the decade.

eg	pressure reading	3.2×10^{-7}	voltage = 3.2V
		1.7×10^{-9}	= 1.7V
		9.0×10^{-5}	= 9.0V

This operation is totally transparent to the user and NO access to alter it via the key pad is available.

6.4 Plotter

Any HPGL (Hewlett Packard Graphics Language) compatible plotter can be connected to a Sensorlab.

For a serial plotter, the supplied nul-modem plugs into the rear of the computer, then the RS232 cable plugs between this and the plotter. The plotter will need to be set for 9600 baud, 8 data bits, one stop bit and no parity.

Depending on the plotter model and the screen display up to eight colours can be used, such an example would be the HP Colorpro 7440A plotter for the TREND mode of MIM.

Plotter output automatically includes the actual time and date the plot was taken, ideal for archiving data in chronological order.

The plotter output is started by pressing the **Alt** and **P** keys.

6.4.1 Technical Details for Plotter

The screen information is drawn using a number of vectors (line drawing instructions). When a plotter output is requested a duplicate set of vectors are instantaneously sent to a spooler file in the HPGL format. This spooler file will normally exist in the RAM (which is extended to 640K for this option) or on a "hard-card" if available. This means that the mass spectrometer can continue scanning without losing data.

This spooler file is then sent to the plotter as a background task not affecting the operation of the mass spectrometer. The data transfer can only start when the plotter is set "on-line".

You can have **both** a plotter and printer attached to a Sensorlab system if required. The plotter output would still be started by pressing the **ALT** and **P**, and the printer would still work from the **Scn Prt** key.

7. ANALYSER HEAD MAINTENANCE

No routine maintenance of the Sensorlab analyser head is required unless it becomes necessary to replace the filament assembly or excessive contamination is present.

7.1 Replacing The Filament Assembly

CAUTION: **Precautions must be taken to ensure clean working conditions. Clean nylon or cotton gloves must be worn when handling any part of the analyser which is immersed in the high vacuum.**

Should finger grease contaminate any part of the analyser, the whole assembly must be cleaned.

The filament in the analyser head can be quickly and simply changed by the user. Spare filaments are available from VG Quadrupoles at the address on the front page of the manual or from the local agent.

Switch off the Sensorlab control unit. Disconnect the multi-core cable from the remote head. Remove the remote head from the analyser by first unscrewing the plastic coupling nut or rotating the wing fasteners (depending on your analyser type) and then carefully withdrawing the remote head from the feedthrough flange, making sure that the feed-throughs are clear of the remote head before removing the head.

Shut down the high vacuum pumps or isolate that part of the system containing the analyser head.

CAUTION: **The instructions which follow do not apply to analysers with enclosed ion source (EIS), see supplementary notes with your shipment.**

Unscrew the nuts and bolts and carefully withdraw the analyser from the vacuum port. Cover the port.

Support the analyser head in a vertical position when changing the filament. Wearing clean gloves, loosen the three M1.6 cheesehead screws clamping the barrel connectors on the top of the analyser to the pin protruding through the filament plate (see Figure on VIII- 59).

Ease off the barrel connectors and gently move the ceramic-shielded wires away from the analyser body to clear the source.

Unscrew and remove the two M1.6 cheesehead screws and washers which clamp the filament assembly to the repeller.

Carefully withdraw the filament assembly axially. Insert the new filament assembly taking care not to damage the delicate source cage.

The filaments are factory pre-aligned and require no alignment or adjustment except in the case of EIS. Replace the two screws to clamp the filament assembly to the repeller and tighten them lightly.

Place the barrel connectors on the pins and tighten the clamping screws

Re-install the analyser in accordance with instructions in section 3.2 using a new copper gasket.

NOTE: All necessary tools, including nylon gloves and a supply of copper gaskets, together with 3 spare filament assemblies, are included in the Filament Tool Kit available from VG Quadrupoles or the local agent.

7.2 Non-Standard Filament Materials

The Sensorlab can be supplied with filament wire of a material other than the standard Thoriated Iridium. The available options are Rhenium or Tungsten.

Thoriated Iridium emits electrons at a much lower temperature than either Tungsten or Rhenium (it has a lower work function) and so requires less current supply to the filament in order to produce the pre-set electron emission current. When using other filament materials, the filament current limit should be increased to provide sufficient emission for control. The filament current limits for filament materials are as follows:- Th 2.2A, W3.1A, Re 3.1A.

The Sensorlab may now be operated normally in accordance with the operating instructions herein.

7.3 Cleaning The Analyser Head

If the analyser becomes contaminated with pump oil or finger grease it may be cleaned as described below. Remove thoriated iridium filament assemblies as the thoria coating can be dislodged if subject to prolonged agitation.

For Faraday analysers only, immerse the complete analyser head in a beaker of clean Arklone 'P', acetone, propanol or trichlorethylene.

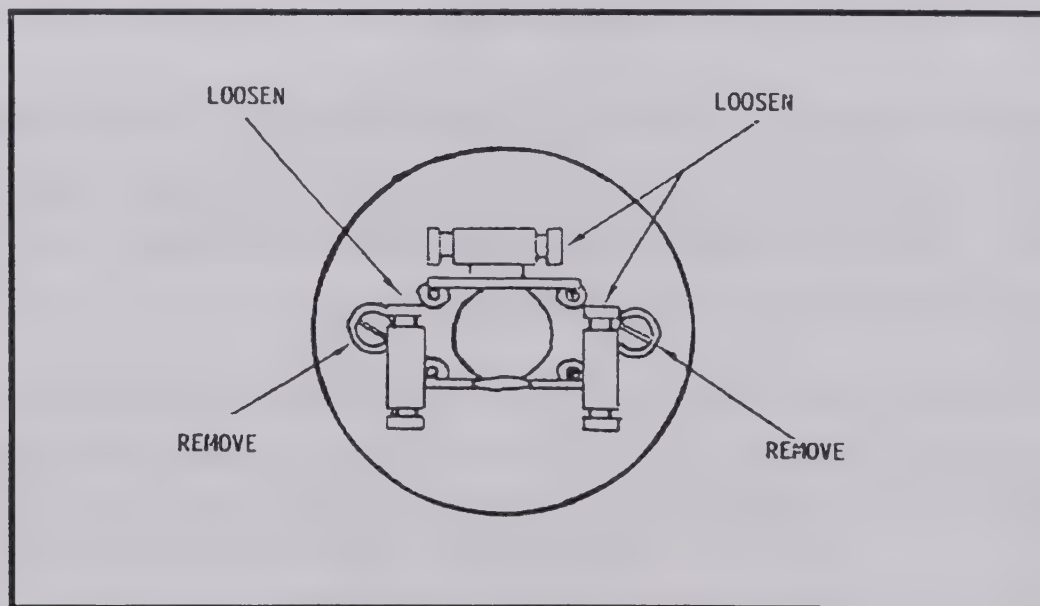
For Dual Detector (SEM) analysers, immerse the filter part of the analyser in a beaker of clean Arklone 'K' acetone or propanol, but **not** the part of the analyser containing the electron multiplier.

Place the beaker in an ultrasonic cleaning bath for 20 minutes.

Remove the analyser from the cleaning fluid and allow excess fluid to drain off. Place the head in a clean drying oven at 80°C for 2 hours.

Use clean nylon or cotton gloves to handle the clean analyser.

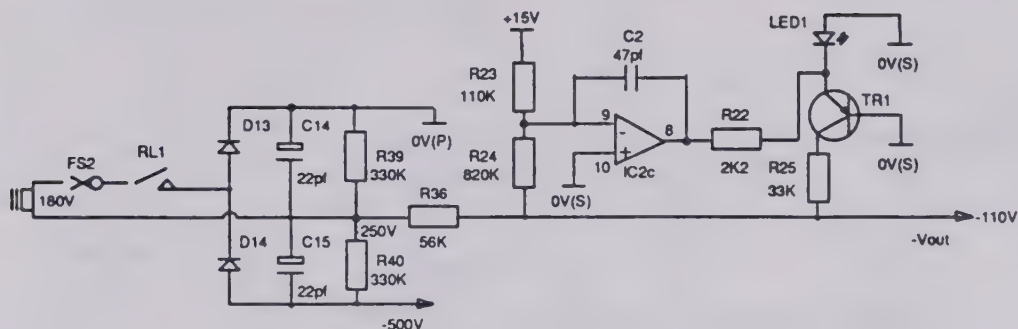
Should the above procedure not remove the contamination, it may be repeated and failing that the analyser head should be returned to the factory for a thorough clean and re-build if necessary. Factory repairs are accompanied by a report when requested to suggest safeguards against repetition.



8. POWER SUPPLY SLOT CARD

8.1 Source Supplies Circuit

8.1.1.1 Parallel Regulator



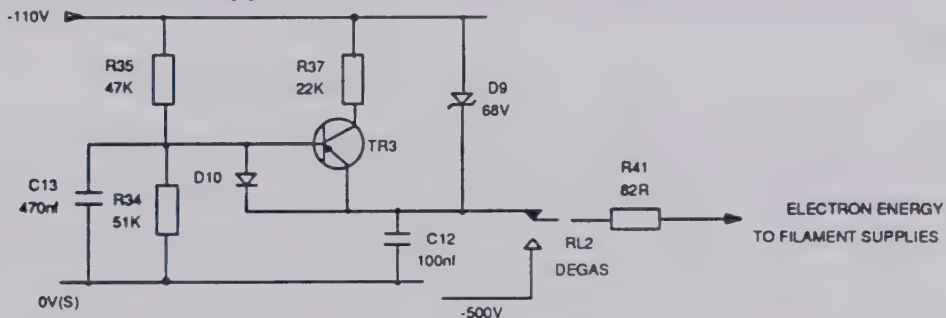
The 180v A.C. is rectified in a standard voltage doubler circuit which gives -250v and -500v unregulated. The -250v is fed to a parallel regulator with R36 being the dropper resistor.

For balance, IC2C pin 9 must be held at 0v. This means that current through R23 is $+15\text{v}/110\text{k}$. The same current flows through R24, hence $-V_{\text{out}}$ is $(+15\text{v}/110\text{k}) \times 820\text{k} = -111.8 \text{ volt}$.

Assume -Vout falls towards 0v. This causes IC2C pin 9 to go positive, hence pin 8 goes less positive, reducing current drawn via TR1 and R35 from R36. This reduction through R36 causes -Vout to rise back to -111.8v.

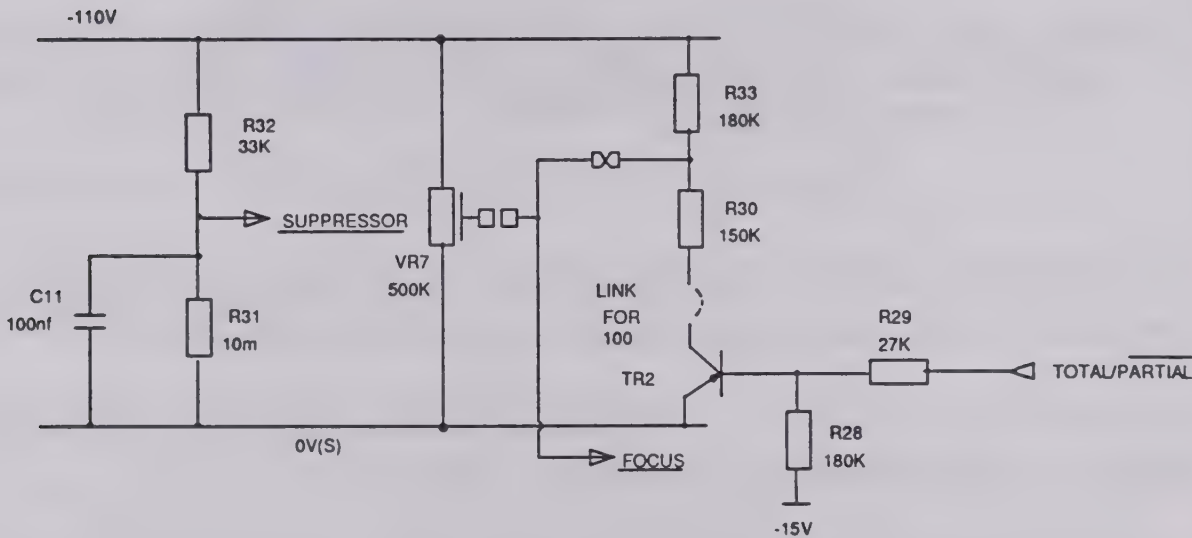
R25 limits the dissipation in TR1. LED 1 will light if IC2C pin 8 goes negative. This will only occur on failure of the regulator because normal operation has pin 8 varying about positive voltages. C2 is for stability only.

8.1.2 Source Supplies



The electron energy voltage is simply buffered from a potential divider network, R34/R35, giving $(-110 \times 51k)/(51k+47k) = -58v$.

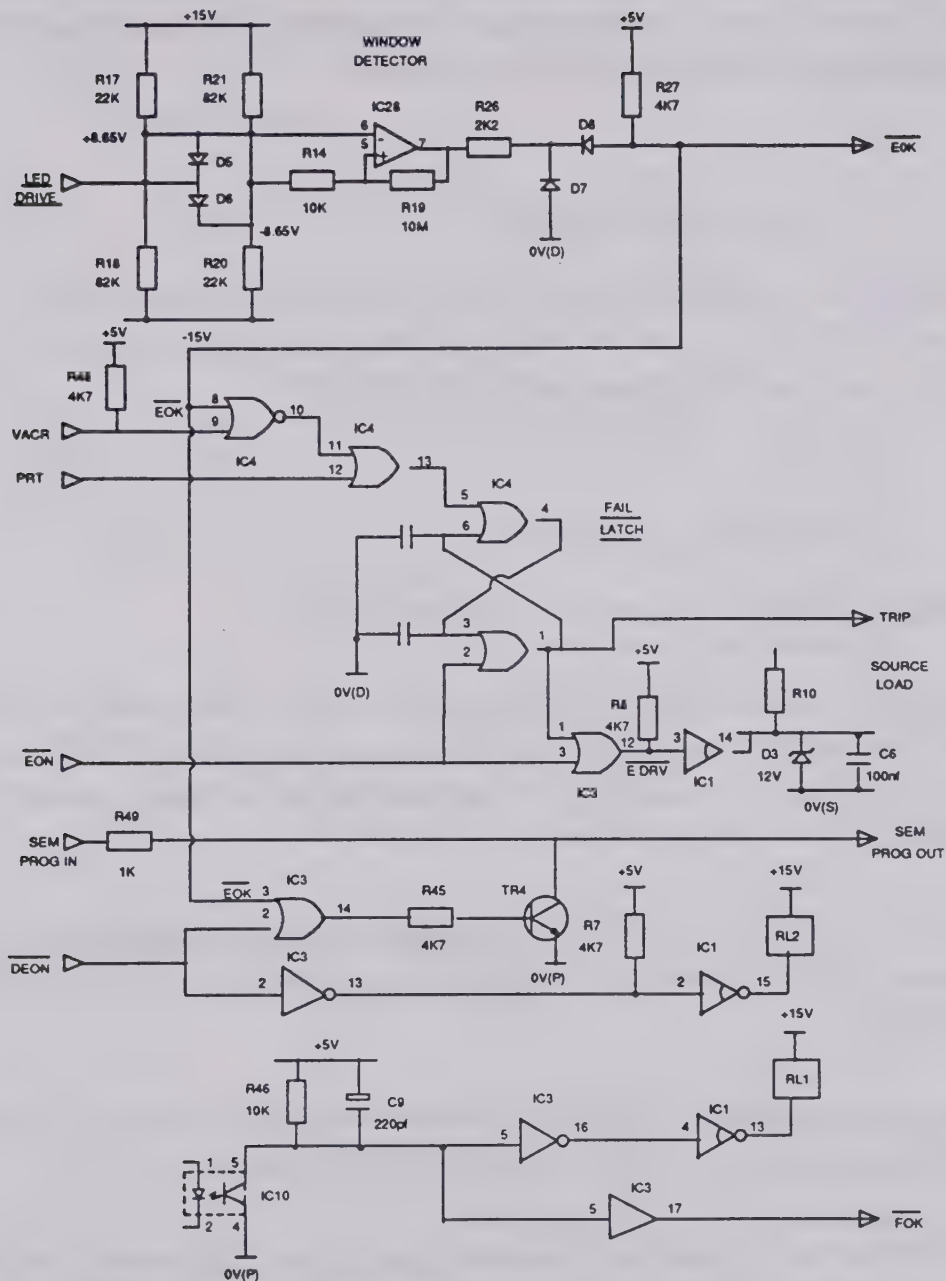
R37 limits dissipation in TR3. D9 is to absorb transients that occur on the lines; eg. during return from degas with -500v Electron Energy.



The suppressor voltage is to all intents and purposes with $\frac{1}{2}v$ of the -110v rail. The resistors just provide extra filtering.

The Focus line is normally tapped down from the -110v by R30/R33 giving about -92v. TR2 is conducting because in partial the drive to R29 is low, hence the base of TR2 is pulled on by R28. During total mode, R29 is pulled to +5v, cutting off TR2. The Focus line now rises to the -110v rail, defocusing the beam, and in conjunction with a new R.F. level, allows all energy present to pass the collector.

8.2 Control Circuitry



8.2.1 Window Detector ($\overline{EOK}$)

As long as the LED drive remains between -8v and +8v, then D5/D6 conduct, and IC2B pin 6 is positive with respect to pin 5. This causes IC2B pin 7 to be at -15v. This pulls down D8 cathode to -600mV (held by D7) and $\overline{EOK}$ is 0v.

If the LED drive goes above +8v, then D5 backs off, and pin 5 of IC2B goes positive with respect to pin 6. The same happens if the LED drive goes below -8v when D6 backs off. When this occurs IC2B pin 7 goes to +15v and raises D8 cathode. D8 backs off, and R27 pulls the EOK line high to +5v. This indicates a failure of the emission control circuit.

8.2.2 Filament Detector ($\overline{FOK}$)

As long as filament current flows, then opto IC7 conducts. This pulls down IC3 pin 5 giving $\overline{FOK}$ low on pin 17. IC3 pin 16 drives the darlington buffer IC1 pin 4 high, calling RL1. This enables the analyser source supplies, and hence source current can flow.

8.2.3 Emission on Actions ($\overline{EON}$)

Prior to enabling emission - ON, the static conditions are:-

PRT high forcing IC4 pin 5 low. With $\overline{EON}$ high, IC4 pin 1 is low, and hence IC4 pin 6. This gives IC4 pin 4 high, and TRIP low. $\overline{EON}$ high also causes IC3 pin 12 high ($\overline{EDRV}$), and darlington buffer IC1 pin 14 pulls the source to 0v. At this point, because no filament current flows, RL1 is de-energised.

$\overline{EON}$ is pulled LOW. This gives $\overline{EDRV}$ low, disabling IC1 pin 14, releasing the source to rise to +12v (caught by D3). The source at +12v causes filament current to flow producing $\overline{FOK}$ low, and RL1 energising.

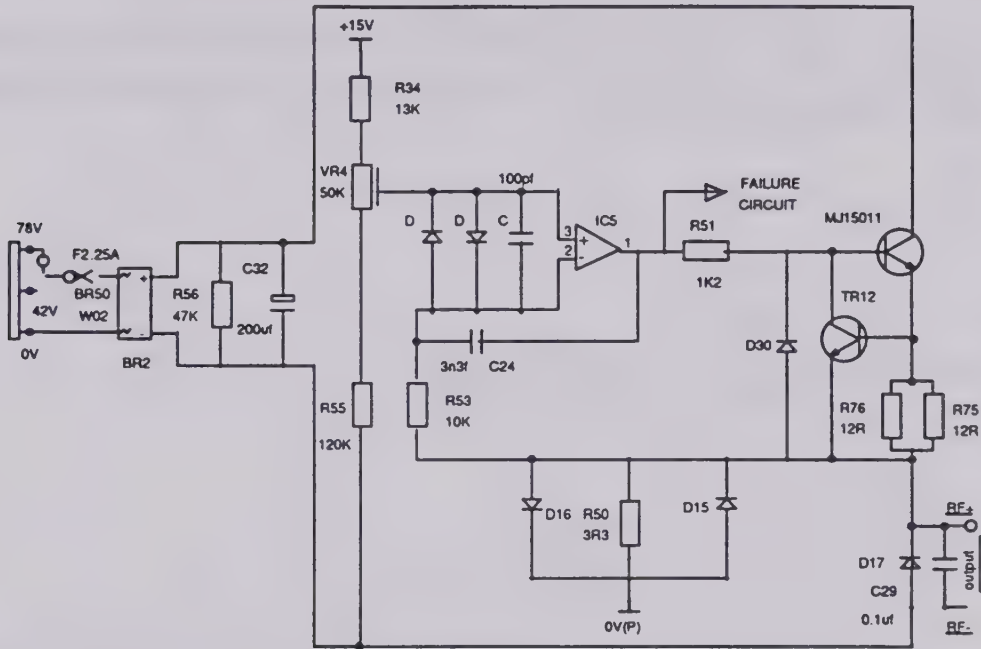
Now normal source stabilisation takes place because source supplies are present. Correct LED drive gives $\overline{EOK}$ low. Providing VACR is low, then IC4 pin 10 is high.

Failure:- PRT can now be pulled low. If emission now fails, and $\overline{EOK}$ goes high, this pulls IC4 pin 11 low, IC4 pin 5 high causing the fail latch to flip. TRIP goes high, pulling $\overline{EDRV}$ high, and source low. This shuts down emission, and the circuit stays this way until $\overline{EON}$ is released. The actions can now be restarted.

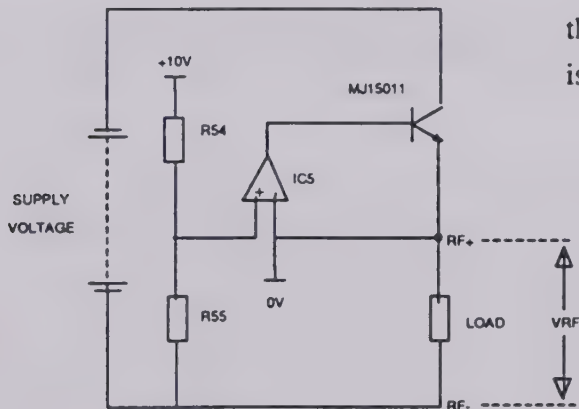
TR4 switches off SEM supplies in the event of emission failure, or Degas ($\overline{DEON}$) by pulling the SEM PROG line low.

Note:- EMISSION ON sequence is $\overline{EON}$ (L) $\rightarrow$ release source to +12v $\rightarrow$ filament current goes to current limit $\rightarrow$ FOK goes low $\rightarrow$ Source supplies enabled (RL1) $\rightarrow$ source stabilised at I.E. level and filament out of current limit $\rightarrow$ $\overline{EOK}$ low.

8.3 RF Power Supplies



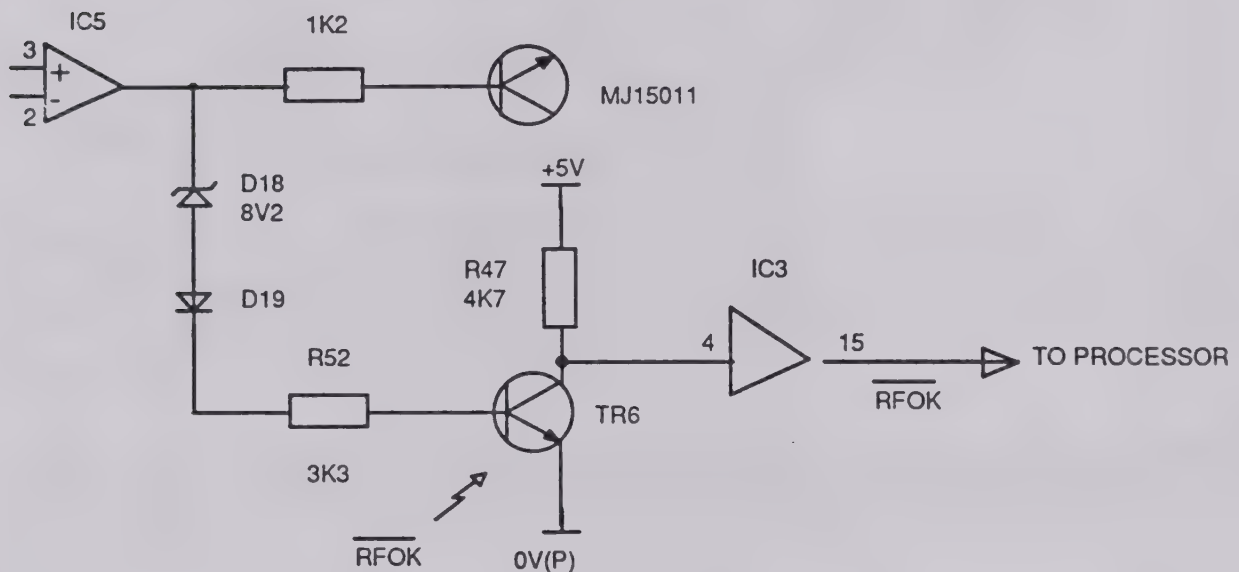
This circuit is best described using the following circuit.



The voltage between the Collector and RF - is constant

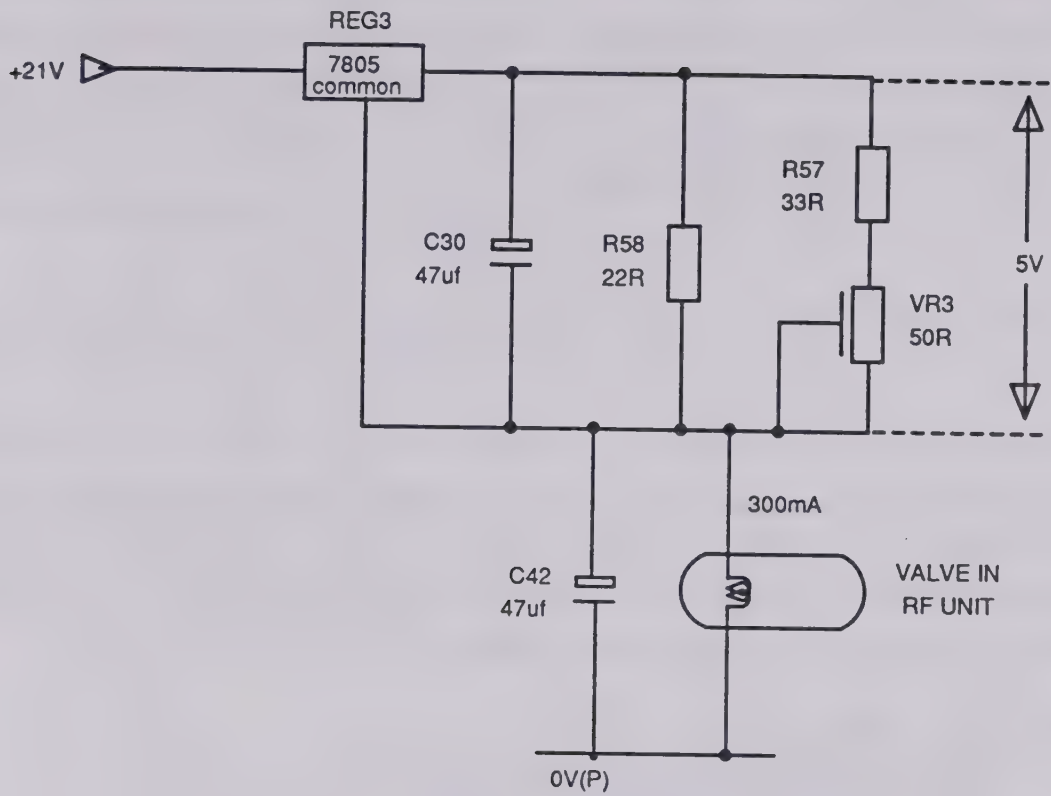
Assume that the RF- falls towards 0V. This means that the collector of the MJ15011 must rise. The non-inverting input of IC5 also rises causing the MJ15011 to conduct heavier, pulling down its collector, and hence pushing the RF- back from where it fell. This is achieved because the OP-amp used 0V on its invert input, and the +15V reference for its non-invert input, even though the RF power supply is floating.

TR12 is a current limit transistor, limiting output current to about 110mA. D15, D16, and resistor R50 are to allow the RF drive to float and reduce pick-up in the amplifier chain, and yet the maximum float is limited to $\pm 600\text{mV}$ by the diodes.



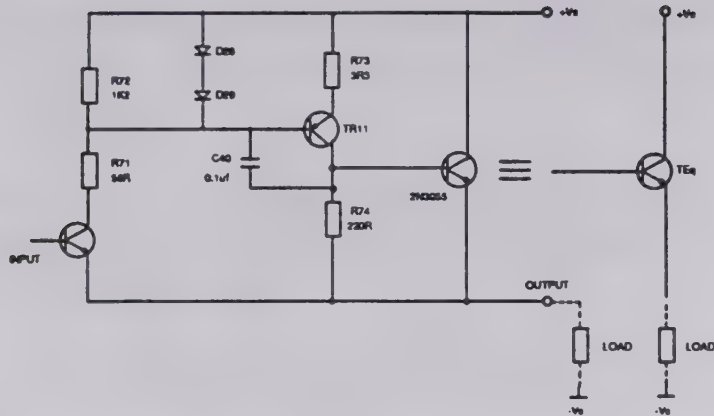
If the drive to the base of the 2N3773 from IC2 exceeds 8.8V (D18 and D19) then TR6 conducts, pulling IC3 pin 4 low, hence $\overline{\text{RFOK}}$ line to the Interface board, and hence the processor unit.

8.4 Valve Heater (200 amu only)



REG3 is an ordinary 5v regulator. It maintains 5v across the load consisting of R57, R58 and VR3. This means that the current through the load can vary between about 144mA and 377 mA. The same current must therefore pass through the valve. It is preset to 300mA for correct operation.

8.5 Emission Regulator

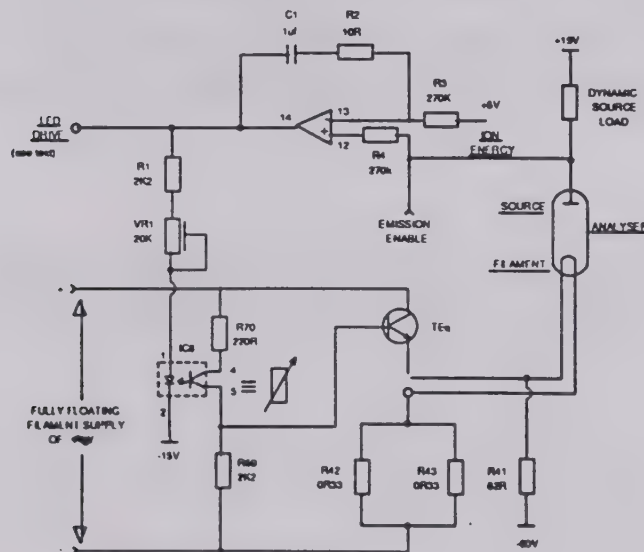


Transistors TR9, TR11, and the filament driver transistor 2N3055 act as a compound single transistor with very high current gain, but unity voltage gain. D28 and D29 act as current regulators limiting the base current to the 2N3055 to about 180 mA. This limits the maximum current to the load to about 8 amp under short-circuit conditions, and no other control.

There are two basic control actions:-

- i) Emission regulation by filament current control.
- ii) Current limiting of a cold, or faulty, filament.

8.5.1 Emission Regulation (Simplified Diagram)

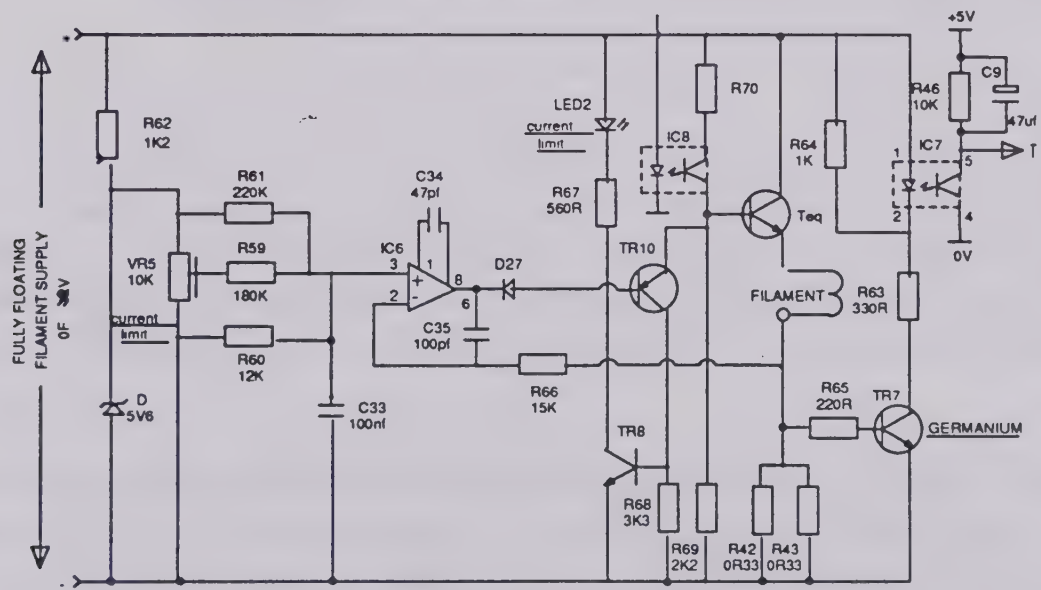


Assume source current is flowing, and it tries to increase. More voltage is developed across the source load, and hence the non-invert input of IC2 will fall. This reduces the current fed via R1 to the opto-isolator IC8. Decrease of opt-isolator diode current causes the transistor to behave like a higher resistance in the bleeder chain R70, IC8, R69 driving the composite transistor Teq. The base current to Teq falls, and hence filament current falls, reducing source current, and hence restoring the conditions to balance.

The value of R15 is adjusted between the limits of 2K2 and 22K so that under normal running conditions the "LED DRIVE" test point is between 0v and -5v.

NOTE: That source current cannot flow until the -60v is applied to the filament connection. This does not stop filament current flowing.

8.5.2 Current Limiter



The non-inverting input of IC6 is the reference voltage against which the voltage across the current sensing resistors is compared. It is derived from a simple zener diode regulated supply.

If the voltage developed across the current sense resistors exceeds this voltage, IC6 output falls, causing TR10 to start to conduct by-passing base drive from "Teq" and stopping any further rise in filament current. VR5 sets this current level to about 3A.

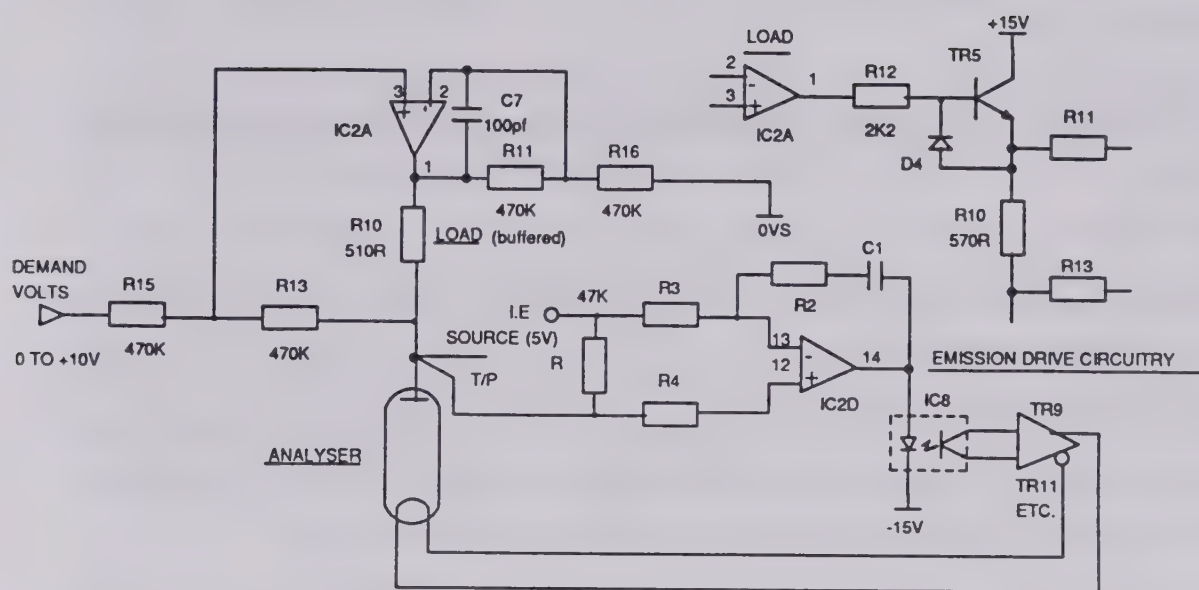
When TR10 current flows, the current flows into TR8 base rather than through the 3K3, and hence TR8 also conducts lighting the "CURRENT LIMIT" LED.

To enable switching of the -60v, TR7 is used. It is a Germanium transistor needing only about 150mV at its base for conduction. As soon as sufficient filament current flows to develop over 150mV across the sensing resistors, TR7 conducts turning on the opto-isolator IC7 causing its output to fall low. This is used indirectly to switch the -60v to the Emission Regulator Circuit.

For correct operation then, filament current must be sufficient to develop over 150mV across the sensing resistors, but not so high as to drive into current limit. Turn-on current is about 1A, and current limit is adjustable between approximately 1.7A and 3.7A.

R44 across the filaments is there for when a filament fails. It bleeds off any charge collected by the floating open filament which may affect the beam, and hence the signal quality.

8.5.3 Variable Emission



For a simple explanation, assume R10, the source load, is 500R, and unbuffered. If the demand input is 1v, and for stable running, the SOURCE must be at Ion Energy (+5v), then R13/R15 junction is sitting at 3v. For balance in the op-amp IC2A, the output must be at 6v in order for R11/R16 junction to sit at 3v. This means that there is 1 volt across R10, hence 2mA flows through it. As long as R11, R13, R15, and R16 are large with respect to R10 then this is the source current for practical purposes.

It can be shown that this holds true regardless of the Ion Energy setting. To reduce the dynamic impedance of the source load during changes (ie. Emission on, or change of demand voltage) a 47k resistor is connected between the source and Ion Energy. This damps any tendency to self-oscillation due to time delays in the analyser and associated drive circuitry.

The load is buffered from the op-amp by TR5, R12, D4, but this has no effect on circuit performance because they are outside the measuring loop.

An increase in demand voltage cause the source to rise towards +15v. This causes increased filament current via IC2D, IC8, TR9 etc. This causes an increase of source current, bringing down the source until balance is again achieved. The reverse occurs for a decrease in demand.

9. RF GENERATOR

100 AMU units

The RF Generator consists of a crystal controlled oscillator, a driver stage, an output stage, the rf amplitude, a $\pm$ constant voltage source, a unity gain differential input stage, and connections for the Total mode.

The oscillator and buffer are three CMOS gates, IC5, the oscillator comprises the crystal, R39, C38 and C39. The other two gates are parallel buffers, L3, C36, C37 and C35 together with the input impedance of the driver stage, TR5, shape the 2MHz square wave appearing on pins 1, 5 and 8, 13 to approximately a sine wave. The driver is powered from the $\pm 15V$ rails only and is decoupled by R37, C31 and R36. The voltage on the TUNE test point controls the base bias current and hence the gain of TR5 and thus the rf drive via the tuned current step-up transformer T1.

The output transistor TR6 has the output transformer primary in its emitter circuit. The output stage is decoupled by C34.

The output transformer, T2, is voltage step-up with two anti-phase secondaries. The two live ends are connected to the rods and the other two ends are connected together via C8 and C11 which pass most of the circulating rf current. It is tuned by the rod capacitance, and fine-tuned by C21.

The rf amplitude control consists of two capacitive attenuators C18, C19, C20, C27, C26, C28. The attenuated rf is rectified by D11 and D12, the resultant negative voltage is fed via R11 and R12 to the virtual earth of IC3 where it is compared to the programme voltage via R32. The resultant amplified error signal is applied via R34 to the base of the driver stage, TR5 thus adjusting and correcting the output rf voltage. The small temperature-compensated negative voltage applied to the cathodes of D11 and D12 by TR2 and VR4 'Diode Offset' is to ensure linear rectification at low levels of rf.

The dc voltages applied to the earthy ends of the transformer secondaries are supplied via two rf filters C6, L2, C10 and C5, L1, C7. The positive dc (0 to +40V) is supplied by a voltage doubler C4, D2, D1 and C2 via R7. The amplifier, IC1 and TR1 is an inverting unity-gain stage which ensures that the positive dc tracks the negative dc with VR2 'Balance' adjusting out any tolerances.

The negative dc (0 to -40) is supplied by a voltage doubler C3, D8, D7 and C14 via R15. The amplifier, IC2 and TR3 is an inverting stage with a gain of 8.3. The exact output voltage is adjusted by VR3 'Resolution'. This adjusts the ratio between the rf and dc voltages.

The differential input stage, IC4 has a zero offset adjusted by VR6 'Scale' and its gain adjusted by VR5 'Mass'. These two trimmers are used to fit the spectrum to the monitor display.

When in 'Partial' mode the TTL input on Pin 6 is low and RLA de-energised. When the Total mode is selected a high TTL level is applied to Pin 6 and RLA is energised. This connects both dc inputs together and to 0V.

D4, when fed from TTL high causes the two DC generator outputs to increase to their maximum, this is for Beam OFF.

9.1 Amplifier

This consists of two stages, a current to voltage stage and a variable gain voltage amplifier.

The current amplifier (IC3) is a FET device with a very low bias current. It has two feedback resistors connected in series with a reed relay to short one of them out. Feedback is arranged with R24, R25 and TR5 to give a voltage gain of three and when TR5, switches "off" a voltage gain of one.

The voltage amplifier (IC2) has an adjustable gain in the range of X3 to X1000 with steps of X3, X10, X30 etc. One of the CMOS switches in IC1 is used to switch a capacitor (C4) in parallel with C5 on the higher current gain range to reduce the bandwidth and thus the noise.

The first stage (IC3) and the zero setting potentiometers are fed from a locally established $\pm 12V$ using the two regulators Reg 1 and Reg 2.

TR4 is used as a local buffer between the Beam Off (BO) signal and the RF generator.

9.2 SEM Supply (D)

This is a programmable negative high voltage supply mounted in the remote head. When the programme is +10V an output voltage of -3,500 volts is produced, as the programme is reduced the output reduces in a linear manner towards zero. When the programme becomes less than 1.1 volts it is switched "off" and the output, after a short delay of 0.5 seconds, is shorted out by a reed delay (RLA).

The blocking oscillator (TR4) drives a step up transformer at a frequency of about 50 KHz and the secondary drives a four stage voltage multiplier (D2, D3, D4 and D5), after smoothing by R2 and C5 it produces a smooth dc output voltage. The current in the feedback resistor (R4) is compared to the current in the input resistor (R10) and the amplified error is fed to TR2 which varies the supply volts of blocking oscillator. TR1 monitors the average current to the output stage via R12 and forms the current limit for the supply.

The other half of IC1 and TR3 form a comparator, delay circuit and relay drive for the output shorting circuit with R8 setting the threshold voltage. R16 ensures the drive to the oscillator is reduced to zero in the "off" condition. REG 1 is used to improve the supply rail rejection when long cables between the remote head and control unit are used. R11 and C10 are to reduce any hum pickup in the programme leads which would otherwise modulate the output voltage. C7 and C13 are to reduce high frequency pickup on the error amplifier input stage of rf from the rf generator and voltage spikes from the output blocking oscillator.

9.3 RF Generator

200 and 300 AMU units

The RF Generator is split into 2 p.c.b.s, one being the main p.c.b. which is permanently connected to the RF generator and head amplifier chassis and the other being the output stage which is soldered direct to the chassis mounted RF output coil leads and the wiring harness.

The RF generator produces two equal amplitude a.c., R.F. voltages at 2 MHz which are in antiphase with each other and are respectively offset by equal and opposite polarity d.c. levels. The ratio of d.c. offset to a.c. amplitude remains a closely controlled constant whilst the overall amplitude is varied in direct proportion to the input program voltage. The two resulting outputs are connected one to one pair of diametrically opposed poles and the other to the other pair of diametrically opposed poles of the analyser. The resulting effect is that of varying the mass pass-band of the analyser in direct proportion to the R.F. generator input program voltage.

9.4 Operation

The operation of the R.F. generator is as follows:

The inverter at pins 10 and 12 of IC1 together with crystal X1.R2.C5 and C6 forms a 2 MHz oscillator, its output at pin 12 is used to drive two parallel output buffer inverters whose inputs are at pin 3 and pin 6. The 2 in-phase parallel square waves are filtered and mixed to an approximate sine wave at the base of TR1 by C2, C4, L1, C1 and the input impedance of TR1. The driver transistor TR1 is powered from the $\pm 15V$ rails de-coupled by R6, R3 and C3. The oscillator runs from the -15V rail and 0V (p) and is de-coupled by R6, C9, R1 and C8. The voltage on the tune test point controls the base bias current and hence the gain of TR1 and thus the R.F. drive via the tuned current step-up transformer T1. The isolated center tapped outputs of T1 at a d.c. potential of -80V provide push pull drive to the common base configured output power transistors TR1 and TR2 mounted on the output p.c.b. The outputs at the collectors of TR1 and TR2, which are connected to L1 and L2 produce 2 antiphase R.F. voltages, any d.c. offset being removed by C13 and C17. These voltages are stepped up by the two chassis mounted air cored coils which are tapped to produce correctly balanced output voltages and tuned to resonance by the dual air gap tuning capacitor.

Feedback for control of the p-p R.F. voltage level is provided at the input of error amplifier IC5. The two capacitive dividers C7, C8, C9 and C3, C4, C5 provide a percentage of the two antiphase output voltages at the two anodes of the diode valve. Whenever the voltages, at either of the 2 anodes goes above 0V (set exactly by the valve offset trimpot VR2) the diodes conduct, negatively charging C3 and C7 to a mean negative voltage equal to a fixed percentage of the p-p R.F. output voltage. When the 2 antiphase signals are mixed at the node of R1 and R2 the a.c. component completely cancels out and a d.c. current proportional to the R.F. amplitude flows into the non inverting input of IC5 the level of this current and hence the p-p R.F. output level is determined by the program voltage on the program test point. As the program voltage is increased the voltage at the non inverting input of IC5 increases causing its output to go positive and produce more R.F. drive. R.F. drive continues to increase until the current flowing from the node of R1 and R2 on the output p.c.b. causes the non inverting input of IC5 to return to virtual 0V, at this point the circuit is regulating and R.F. output is directly proportional to program input. The tune test points are used to adjust for resonance of both the transformer T1 and the output coil. The nearer to resonance both these tuned circuits are, the less amount of drive voltage required from the output of IC5, hence at resonance this voltage will be at a minimum. R35 and LED 1 provide a rough indication of the tuning. When LED 1 is lit the output of IC5 is positive. Whilst under normal tuned circumstances this volt will always be negative, the LED hence indicates an untuned R.F. generator.

Program input voltage from the control unit (as described above) appears at pins 9 and 10 of SK3 of the main R.F. generator p.c.b. This is the differential common mode signal rejecting input of the unity gain input amplifier IC4. A small offset voltage is added to the input R32 via Trimpot VR6 (SCALE) and R30, R31 divider. The gain of IC4 is closely controlled by the high stability resistors R25, R32, R33 and R34 whilst immunity to high frequency transients is provided by C15 and C19. The output of IC4 is divided via VR5 (MASS) VR4 (RESOLUTION) and R20 into two output signals, one at the junction VR5 and VR4 which provides program for R.F. amplitude control and the other at the wiper of VR4 (RES) which provides program for control of the d.c. components of the output. The divider therefore provides a constant ratio between R.F. and d.c. programs which may be adjusted via VR4 (RES).

The positive and negative unregulated d.c. is derived from the R.F. outputs of TR1 and TR2 on the output p.c.b. Positive d.c. is derived via R3, R4, a.c. coupling capacitors C18 and C20 full wave bridge rectifier D1, D4, D5, D8 and referred to +15V, and smoothing capacitor C16, whilst negative d.c. is derived via R3, R4 a.c. coupling capacitors C19 and C21 full wave bridge rectifier D2, D3, D6, D7 referred to -80V (-135V) and smoothing capacitor C14.

The regulated negative d.c. level is set by the program input voltage at the wiper VR4. This positive voltage produces a current through R18 causing the inverting input of IC12 to rise and produce a negatively going error signal at its output. This turns off TR6 via R13 and allows the collector of TR6 to be pulled negative by R26. As the collector of TR6 becomes more negative the voltage across the junction of R16 and R18 is brought to rest at the virtual 0V. C10 is provided for stability.

The positive DC is derived by the same method, but in this case the error amplifier input is provided by the negative DC supply at R22. This causes the voltage at the inverting input of IC3 to go negative causing its output to go positive thus turning off the shunt regulator TR5 and allowing its collector to be pulled up by R27. As the potential at the collector of TR5 continues to rise, voltage across R21 increases moving the inverting input of IC3 positive. The circuit reaches equilibrium when the wiper of VR1 is brought to rest at 0V by adjustment VR1 the positive and negative voltages are exactly balanced.

The 2 DC offsets are applied to the RF output coils via 2, 2nd order passive low pass filters L1, C2 and L3, C21 which attenuate RF to the DC supplies. C10, C11 and C12 act as an AC earth for the RF coils whilst allowing the DC offsets to be applied directly to terminals C and D of the output coils.

9.5 Digitally Controlled Head Amplifier

The head amplifier takes its output from either a Faraday collector or a semiconductor secondary emission multiplier, the latter having the ability to produce a high gain current signal before application to the amplifier input.

The amplifier is split into 2 PCBs these being the current amplifier (input stage) and the voltage amplifier (output stage). The current amplifier, operating at very low signal levels (ie 10^{-11} amps of input for 1V of output at the highest gain) is most sensitive to noise and has to be screened inside a metal case to avoid spurious hum and noise, whilst the less sensitive voltage amplifier remains accessible for adjustment of pots.

9.6 PCB1 Current Amplifier

The input from the analyser appears at a common connection between the two reed relays RLB and RLC on the current amplifier PCB1. The input PCB can be set to one of three gains. With RLA open or closed, RLB open and RLC closed. The highest gain is selected and the signal is routed to the inverting input of IC2 (a 310J operational amplifier module). IC2 has a maximum input bias current of 10^{-14} Amps.

Feedback resistor R10 (1×10^{11} ohms) produces a gain of 1 volt output for 10 pico Amps input (normally expressed as 10^{-11} Amps/Volt. R8, R9, C6, R7 and C5 provide low pass filtering for noise rejection. Temperature compensation is also applied to minimise offset voltages.

With RLA open, RLB closed and RLC open the input is routed to IC1 an operational amplifier. The gain is set by the feedback resistor R1 (1×10^8 Ohms) producing a gain of 10^{-8} Amps/Volt. The cut off frequency of the amplifiers of set by R1 and C4.

9.7 PCB2 Voltage Amplifier

In addition to the voltage amplifier this PCB contains circuitry for temperature compensation of the 310J; gain select logic; relay drives; zero set facilities for 10^{-11} , 10^{-8} and 10^{-5} amps/volt current gains; and $\pm 12V$ supplies used by both the voltage amp and RF generator.

The $\pm 12V$ power supply is derived from the $\pm 15V$ power supply on the control unit PCB. DC inputs are de-coupled by C1 and C2 and supply IC1 and IC2 which regulates to $\pm 12V$. C3 and C5 suppress high frequency transients on the supply lines.

10^{-8} and 10^{-5} Amps/Volt current amp gains require zero adjustment. These adjustments appear at the input of IC6 in the form of small dc input voltages. The 10^{-8} A/V adjustment is provided by RV4, connected to 12V and the pot chain R56 and R53 capable of producing IC6 dc input voltages between 100mV at the junction of R53 and R49. Any small difference between 10^{-8} A/V and 10^{-5} A/V zeros are compensated by RV5 and R48 which supply current to the junction of R49 and R53. RV5 is effectively switched in and out by TR11 (controlled by the gain select logic). When TR11 is switched on, nearly all the voltage is dropped by R39 and R38 causing a small voltage near zero to appear across RV5 rendering RV5 ineffective (10^{-8} zero) whilst the TR11 is switched off 10V

appears across RV5 allowing the fine adjustment of the 10^{-5} A/V zero to be effective. Remote zero adjustment is provided at the junction of R49 and R53 through R50, R54 and R55.

Depending on the gain selected either RLA or RLB contacts will close allowing either IC1 or IC2 of the current amp to be inputted to IC6 whilst C7 and C8 are switched to provide noise filtering. The gain of IC6 is set at 20 by R40, R41, R49 and R53 together with input resistor R2 or R7 on the current amp pcb.

IC6 output is fed to the inverting amplifier IC7 which has an input resistance of 10K (R42) and a feedback resistance which can be switched by solid state CMOS analogue switches (5) and (6) to either 1M, 100K (1M/110K) or 10K (1M/10K) producing respective voltage gains of 100, 10 or 1. The output of IC7 is connected to the unity gain inverting output amplifier IC8 whose gain may be reduced to zero by switching from (3) and (4) open to (3) open (4) closed.

Digital inputs G0, G1 and MULT/FARADAY control the solid state analogue switches in IC4 and IC5 selecting the voltage gain of the cascade IC6, IC7 and IC8 G2 and G3 digital inputs control the relay drive transistor stages, TR1, TR2, TR3, TR4, TR5, TR8 and TR9 which switch the current amplifier relays RLA, RLB and RLC on the current amp pcb and RLA and RLB on the voltage amp pcb to produce the desired gain as shown in the table contained on the schematic diagram M401-7C.

9.8 Power Supply for the Secondary Emission Multiplier (SEM)

The gain of the SEM is set by the amount of voltage applied to it. This voltage is adjusted by the SEM voltage control and is variable between -600V and -3500V.

Program voltage (0-10V) to the multiplier PSU is supplied from the 10V reference through pot chain R47, Mult Program Pot and R183. SEM mode is selected by SW6/b whilst RLA2 and RLB4 contacts are arranged to prevent operation in Degas and no filament current modes.

Supplied with 0-10V analogue program input and $\pm 15\text{V}$ the SEM power supply produces a 0-3500V output as follows:

Controlled by the output of the error amplifier IC16 via R10, TR4 supplies drive current to the oscillator C5, R11, R12, T1, T2 and TR3, whilst current limit protection is provided by current sense resistor R13 and TR2. Oscillating at about 80 KHz the oscillator generates an ac voltage which is controlled by the amount of drive from TR4 and is stepped up by transformer T2. The output of T2 is rectified and multiplied by the voltage multiplier C7, C8, C9, C10, D6, D7, D8 and D9. The output is de-coupled by R14 and smoothed by C11, R16 provides feedback to IC1b non-inverting input which is balanced with respect to the inverting input at 0V by the program input through pot chain R1, R2 smoothed by C1 and fed to the inverting input of IC1b via R6. C2 and C8 control the speed of error amp response whilst D1 limits the negative voltage at the non-inverting input of IC1b.

Schmitt comparator IC1a has its hysteresis and switch level set to about 1.45V rising and 1.15 volts of falling program by R4, R5 and R7. As program volts fall below 1.15V (which only occurs in degas, no filament current or the Faraday mode) the output of the comparator saturates positive causing the inverting input of IC1b to go positive through D2. This produces a negative error signal at the output of IC1b, turning off drive to TR4 and reducing the output to zero volts after a time set by R15, R16, the load and C11. After the time constant of R9, C3 and switch level set by D5 which is longer than the time taken for the output to reduce to zero under no load conditions TR1 turns on energisers RL1, closes contacts RL1a. This shorts the output via R15 and R17 to earth ensuring no voltage at the output in Faraday, degas and no filament current modes of operation.

9.9 Pole Bias

An addition has been made to the RF electronics (for units over 200 amu) such that an internally set Pole Bias is applied to the quadrupole rods. In order to see whether your instrument has this remove the RF box cover and look for a variable resistor in place of C15. The important parameters to note are:

1. The Ion Energy is now set to 7eV nominally.
2. Pole bias is not applied in RF only (TOTAL) mode.
3. The emission current levels in PARTIAL and TOTAL have not changed.

In order to measure the DC balance and Pole Bias setting the following procedure needs to be used:

Set the Pole Bias to 0V with respect to ground. This is measured on the test pin adjacent to the Pole Bias trimpot. Balance the DC's using VR1.

Adjust the Pole Bias trimpot whilst monitoring the Pole Bias voltage to give a measured -2V for the standard stainless steel source and -3V for the platinum source.

When Pole Bias has been set up the DC voltages applied to the rods will not be balanced.

10. APPENDIX A - GLOSSARY OF VACUUM TECHNOLOGY

PARTIAL PRESSURE:

is the contribution that each component gas makes to the total pressure of the system and is expressed directly in millibar, or in parts per million (ppm). The partial pressure of a gas is obtained by measuring the height of the appropriate peak on the mass spectrum.

TOTAL PRESSURE:

is the sum of the partial pressures.

MINIMUM DETECTABLE PARTIAL PRESSURE:

is the smallest component pressure that the spectrometer can detect.

MAXIMUM OPERATING PRESSURE:

is the highest total pressure at which the instrument may be safely operated.

RESOLUTION:

is a measure of the instrument's capability of separating adjacent mass peaks. For example, 10% valley resolution means that the valley between two adjacent peaks of equal height and separated by one mass unit will be 10% of the height of either of the peaks.

AMU:

Atomic Mass Unit, for example from mass position 27 to 28 is 1 amu.

SPAN:

range of scan. For example, if it is required to scan from mass 28 to 32, set start mass to 28 and use a mass window of 4 amu to give last mass of 32.

BAKEOUT:

is a technique used to obtain low background pressures and a clean vacuum system and involves raising the temperature of the system to (say) 250°C for several hours while under vacuum.

EMISSION:

is a measure of the total electron current leaving the filament. (Hence linked to sensitivity of instrument).

LOW WORK-FUNCTION FILAMENTS:

emit electrons at lower surface temperatures than the tungsten filaments and are used primarily where samples may be subject to thermal reaction.

IONISING CURRENT:

is the part of the emission which causes ionisation within the ion source by electron impact.

PARTS PER MILLION (PPM):

is a measure of concentration expressed as a fraction of the total pressure (taken as 10^6 parts).

BASE PEAK:

Largest peak in spectrum of a pure component.

CRACKING PATTERN:

Tabulation of relative peak heights in spectrum of a pure component. (Usually written using 100 for height of base peak).

RELATIVE SENSITIVITY:

Relative height of a base peak for particular component compared to that for reference compound (often nitrogen) at the same partial pressure.

FORELINE TRAP:

A cylinder filled with activated alumina which absorbs oil vapours typical of those generated by rotary vacuum pumps. When placed in the backing line of a diffusion pump or between a roughing pump and the vacuum system, it reduces backstreaming hydrocarbon contamination to negligible levels.

TORR:

A unit of pressure equivalent to one millimetre of mercury.

MILLIBAR (mb):

A unit of pressure. One atmosphere = 1013 millibar. This is the unit now accepted by the EEC as the standard for vacuum measurement (1 millibar = 0.75 torr).

PASCAL:

A unit of pressure equal to one Newton per square metre.

COLD TRAP:

A cylindrical vessel containing a flask filled with liquid Nitrogen, placed immediately up-stream of an oil diffusion pump. Vapours in the system and most important, oil backstreaming from the pump condense on the cold surface, thereby reducing system contamination. Effective protection against backstreaming is obtained from the cold traps without the use of liquid Nitrogen, the trap acting as an optical baffle. The surface of the flask is polished to reduce radiation losses. There are special techniques for filling cold traps with liquid N₂.

BACKSTREAMING:

is the migration of vapours under molecular flow or near molecular flow conditions against the apparent direction of pumping or gas flow.

MOLECULAR FLOW:

is the condition of gas transport where the mean free path of the molecules is such that collisions occur with the walls of the vacuum vessel rather than between molecules. The result is that molecules can travel in the opposite direction to the bulk gas flow. Pressures when molecular flow occurs, are typically below 10⁻⁴ torr. There exists an indeterminate region between 10⁻² and 10⁻⁴ torr where an unpredictable mixture of viscous and molecular flow occurs. Protection against backstreaming should be provided in this region where appropriate.

VISCOUS FLOW:

is the condition of gas transport where the mean free path of the molecules is such, that collisions occur between molecules rather than between a molecule and the vessel wall (except of course for molecules at the wall). The result is that all molecules travel with the bulk gas flow. Viscous flow conditions exist at pressures above 10⁻² torr.

DIFFERENTIAL PUMPING:

is a technique whereby any part of the vacuum system is maintained at a higher pressure than another, by restricting the pumping speed for the gas from that high pressure part. For example, if gas flows into a mass spectrometer source at a given rate Q and the pumping speed from the source is S then the pressure in the source.

$$P_s = \frac{Q}{S}$$

If the gas then flows through an analyser region where a lower pressure is required to be maintained to minimise ion-molecule collisions and the pumping speed from that region is $10s$ then the pressure P_A will be

$$P_A = \frac{Q}{10s} = \frac{P_s}{10}$$

thus providing a pressure differential between the two regions of 1 : 10.

Several stages of differential pumping may be used in some cases.

ION:

is an atom or molecule which is charged. This charge may result from one or more of the electrons being stripped from the neutral atom or molecule (the usual result of electron bombardment) in which case the net charge is positive; or it may result from the capture of an electron by the atom or molecule resulting in a net negative charge. The latter process (about 1 in 10^4 ions produced are negative) except for a number of molecules which have a high affinity for electrons (e.g. Chlorine).

OPERATING TEMPERATURE:
15°C to 30°C

RELATIVE HUMIDITY:
90% non-condensing maximum

EXTERNAL CONNECTIONS:
Alarm relays (2) rated at 240V, 1A
Analogue inputs (2), 0 to 10 V from external equipment. Data recorded and displayed in a similar manner to mass spectral data.
Chart recorder output
Vacuum Interlock

MOUNTING:
19" rack mounting, 3U high
Bench mounting or floor standing in outer case

WEIGHT:
12 Kg

OPTIONS

ANALOGUE OUTPUTS (10)
0 to 10 V programmable to follow any signal variation of any mass peak.
Two high resolution outputs (2.5 mV per step) plus eight 8-bit DACs (40 mV per step)

INTERFACES
IEEE488 for bi-directional communications with host computer.

PRINTER
Epson or Okidata. Others, including colour, on application or see Data Sheet 024.

MULTIPLEXER (MP8X)
Control up to 8 analyser heads from single programmable control unit. Linking of MP8X units allows unlimited number of analysis points, ask for Data Sheet 022.

12. APPENDIX C - GENERAL PRINCIPLES OF OPERATION

The Sensorlab analyser comprises three sections: the ion source, the quadrupole analyser and the ion detector.

The construction materials are type EN38E(316) stainless steel, alumina ceramic and thoria filament with Nilo-K filament support wires, and copper filament leads.

THE ION SOURCE

Gas atoms or molecules present in the source are subjected to bombardment by electrons generated from a hot wire filament which have been accelerated by the potential difference between the filament with its cylindrical Electron Repeller held at -110V with respect to ground and the cylindrical Source Cage held at approximately 7V with respect to ground. The filament current is normally 1.7A and that level is feedback controlled to give a constant filament to source cage current of 1.45mA.

The nominally -60 volt electrons, strip an electron from the neutral atom or molecule thus leaving it positively charged (charge= $+e$). In some cases, two electrons may be stripped off the neutral leaving it 'doubly charged' (charge= $+2e$).

The positive ions, formed at the cage potential of approximately 7V are extracted from the source and injected into the analyser by a potential of approximately - 110V applied to the Focus electrode.

THE QUADRUPOLE ANALYSER

The analyser comprises four accurately ground stainless steel rods aligned to fine limits in an alumina collar. Opposite pairs of rods are electrically connected and to each pair is applied a combination of RF and dc voltages, the phase and sign of the potentials being opposite for the two pairs of rods.

An ion entering the electric field generated by this system undergoes oscillations in a trajectory which is either stable or unstable depending upon the voltages (both RF and dc) applied to the rods and the mass of the particular ion being considered. A stable trajectory is defined as one where the path of the ion remains wholly within the physical constraint of the analyser so that the ion reaches the collector; an ion on an unstable trajectory will collide with one of the electrodes or the analyser

housing and be neutralised and therefore will not reach the collector. The ability of the mass filter to differentiate between masses is called the resolution of instrument and is determined by the ratio between the RF and dc voltage amplitudes. If that ratio is kept constant while the amplitude of the voltages is increased linearly with time, then the mass spectrometer is tuned sequentially and linearly with time to adjacent masses with increasing mass number (that is 1,2,3 100) and the resolution of the instrument remains constant over the whole scanned range.

This process is called a mass scan and the read-out of peaks thus obtained is called a mass spectrum.

The resolution of Sensorlab is such that adjacent peaks of equal amplitude are separated by a valley of at most 10% of their height. If the dc component is switched off the resolution of the filter is reduced to zero and all masses are transmitted to the collector thus giving a measure of the total pressure of the system.

THE FARADAY COLLECTOR

The Sensorlab collector is a Faraday plate screened from the source and filter supply leads by an earthed shield. A further electrode is present on a 100F analyser, which is kept at - 110V is mounted immediately above the Faraday plate and its shield, and acts both as an electron shield, preventing electrons from the filament from reaching the collector, and as a secondary electron suppressor ensuring that any electrons generated by ions arriving at the collector are returned to it so eliminating possible errors in ion current measurement.

THE SEM COLLECTOR

This is a multiplier mounted off-axis so that neutrals and photons from the hot filament are not detected. The output electrons are collected and conducted through the central pin of the vacuum feedthrough and finally to the amplifier. The multiplier is air stable and provided the output current is kept low and it is not operated above 10^{-5} torr it has a long life expectancy.

It is recommended that the SEM is not operated above 2×10^{-7} mb which corresponds to a current of $1 \mu\text{A}$. The source is said to have a sensitivity of 5×10^{-4} A/mb, so at 2×10^{-7} mb gives a signal $(5 \times 10^{-4} \times 2 \times 10^{-7}) = 1 \times 10^{-10}$ A.

The SEM detector is operated such that it has a gain of 10^{-4} , and so $1 \times 10^{-10} \times 10^{-4} = 1 \times 10^{-6}$ A or 1μ A. The SEM can be used above 2×10^{-7} mb but the SEM voltage must be reduced accordingly.

Further information on Quadrupole theory is available on Technical Information Sheet 02.439.

13. APPENDIX D - RELATIVE SENSITIVITY FACTORS FOR 5" FILTE QUADRUPOLE ANALYSERS

To arrive at a relative sensitivity factor for a given gas the user needs to know the ionisation efficiency relative to nitrogen, the transmission of the quadrupole filter relative to nitrogen (measured in Faraday mode to eliminate mass discrimination effects in the multiplier) and the gain of the multiplier (if in operation) relative to the gain for nitrogen (it is usual to calibrate the multiplier with nitrogen ($m/e = 28$) at a gain of 10^4).

The relative sensitivity factor S_{rel} can be calculated as follows:-

$$S_{rel} = I \times T \times G$$

where I = relative ionisation efficiency

T = relative transmission factor

G = relative gain in multiplier mode

Obviously in Faraday:

$$S_{rel} = I \times T$$

The value for I can be approximated from Fig 1, which shows National Physical Laboratory data for ionisation efficiencies for different gases. The value for I can be approximated by:-

$$I = 0.0491 N_e + 0.207$$

Where N_e is the number of electrons per molecule of the gas.

T , the relative transmission factor can be seen in Fig 2. These data were partly accumulated recently and partly from analysis of test data. The data for high masses ie 28 has been collected from over 35 analysers. Fewer have been used for the low mass data. The shaded region covers the spread of sensitivity of our analysers, the worst errors occurring at minimum and maximum mass. Even so, at mass 200 there is only a spread of a factor of 5, which is not that unreasonable taking the manufacturing tolerances etc, into account. At mass 2 the spread factor is 2.5. A value for T can therefore be read from this graph with an idea of the error that can be associated with it. For more

accurate work the individual user needs to calibrate the mass discrimination of the filter by measuring the peak height of a gas with a known cracking pattern. Note also, that the data given are for mass resolution of 1 amu with 10% maximum valley between peaks. If this criterion is not met then the transmission of the filter will vary, particularly at high and low mass.

G, the relative gain is measured by comparing the peak heights on complimentary Faraday and Multiplier spectra over the range 1-200 amu. A set of results can be seen in Fig.3. The data does not fit a simple M- function but a smooth curve has been drawn through the data. This data can be used to obtain a value of G.

For example, to calculate a value of Srel for Xenon (mass = 131, atomic no = 54):-

$$I_{xe} = 0.0491 \times 54 + 0.207 = 2.86$$

$$T_{xe} = 0.08 \text{ to } 0.28$$

$$G_{xe} = 0.22$$

$$S_{xe} = 0.05 \text{ to } 0.18$$

$$S_{xe} = 0.12-0.06$$

Hence a value of 0.12 can be used as a reasonable approximation. A peak measured at mass 131 must be divided by 0.12 to correct the peak height.

IONISATION EFFICIENCY RELATIVE
TO NITROGEN

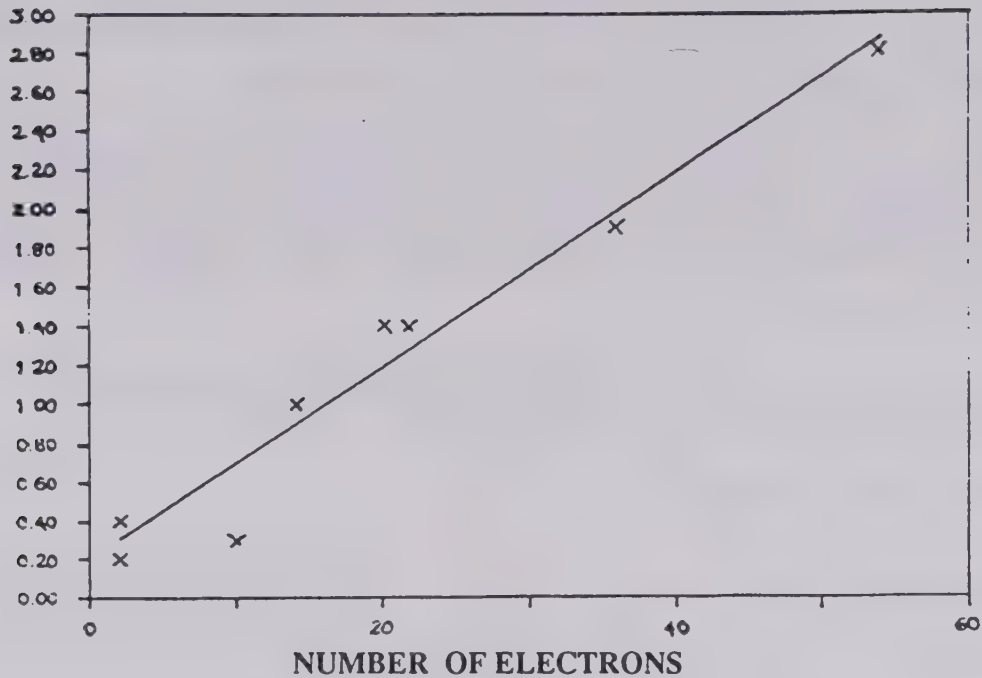


FIGURE 1

QUADRUPOLE TRANSMISSION 5" FILTER DATA
RELATIVE TO MASS 28 (NITROGEN)

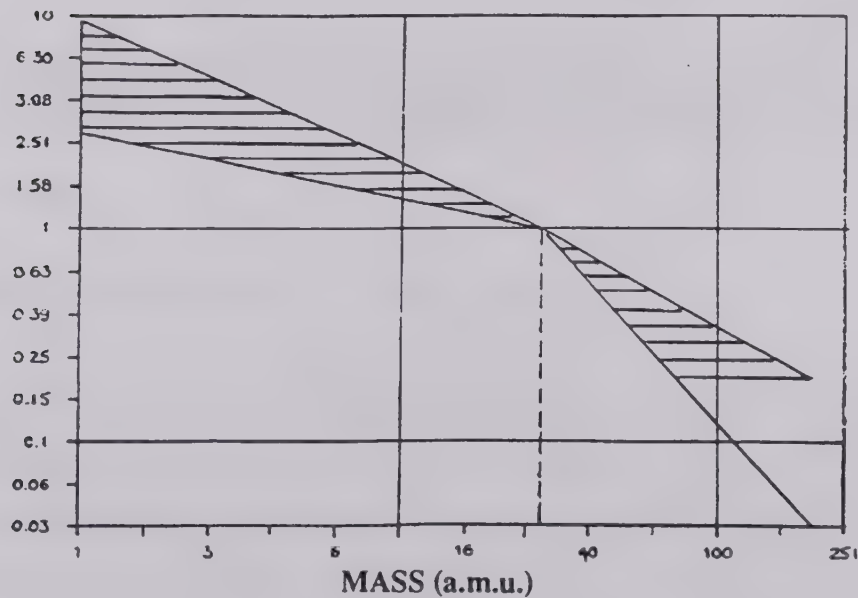


FIGURE 2

SENSITIVITY OF ELECTRON MULTIPLIER RELATIVE TO FARADAY CUP (NORMALISED AT MASS 28, NITROGEN)

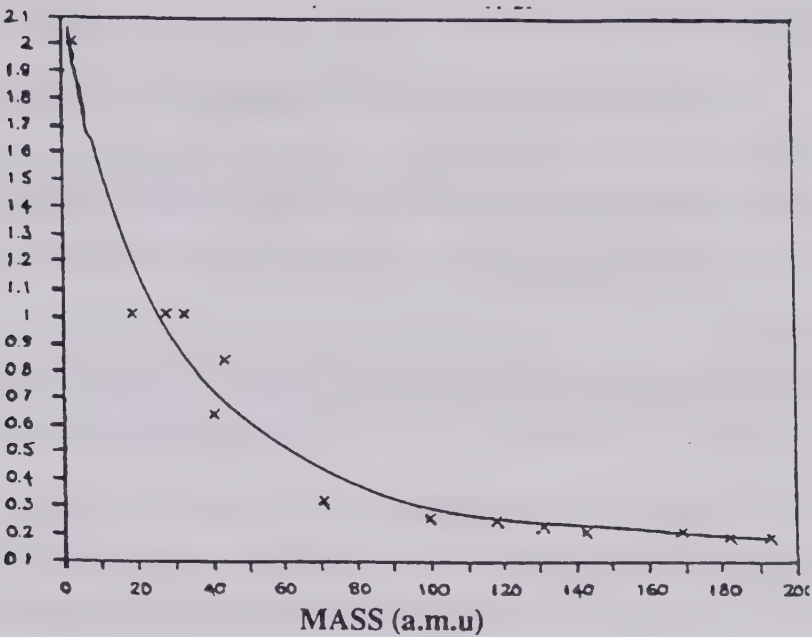


FIGURE 3

14. APPENDIX E - AUTOMATIC LIBRARY SEARCH

Three stages are used in library searching.

- i) An initial short listing to separate a management list of viable compounds.
- ii) A Linear regression to establish the quantitative amounts of each compound.
- iii) A statistical validation.

The initial short listing is based on Bayes Postulate ('without a prior knowledge all options are equi probable ¹') probability assignment. The method is best explained by examples.

If you have a mass present and only one compound in your library has peak at this mass, then you are certain that the compound is present. (It has a probability of 1). If you have a mass present that 3 compounds have (C1, C2 and C3) then the possible viable combinations are:-

C1
C1 + C2
C1 + C3
C2
C2 + C3
C3
C1 + C2 + C3

This is where the Bayes Postulate comes in, as all the combinations are equi probable.

C1 exists in 4 out of the 7 possible combinations so that

$$\Pr(C1) = \Pr(C2) = \Pr(C3) = \frac{4}{7}$$

The Bayes Postulate probability assignment does not take into account information about the shape correlation of the observed spectrum and library cracking patterns. A shape correlation metric is defined as the normalised dot product of the cracking pattern and observed spectrum.

The cracking pattern of a compound can be represented as a vector **CP** whose dimensions is 200 for a 200 amu instrument. The observed spectrum can also be represented as a 200 dimensioned vector **S**. The normalised dot product is simply

$$\frac{\mathbf{C.P.S}}{(\mathbf{CP.CP} \times \mathbf{S.S})}^{1/2} \quad (1)$$

The normalised dot product is constrained to the range 0.0 - 1.0.

The initial short listing evaluates the Bayes Postulate probability and the shape correlation normalised dot product. The larger of these 2 values is used as a ranking for each member of the library. The top twenty compounds are then used in the second phase of the search - the linear regression.

The linear regression is based on the paper by Tunnicliffe and Wadsworth ⁽²⁾. A brief explanatory note is given below. If from the first pass 2 compounds with cracking patterns **CP1** and **CP2** are deemed to make up to make up the observed spectrum **S**. We can represent spectrum **S** as a linear combination of the 2 cracking patterns.

$$\mathbf{S} = \mathbf{a} \cdot \mathbf{CP1} + \mathbf{b} \cdot \mathbf{CP2} \quad (2)$$

The mathematical problem becomes one of choosing a and b to provide the best match. The method used to obtain the best match is to mathematically choose a and b so that the sums of squared differences between observed ⁽⁵⁾ and synthesized spectrum ($a \times \text{CP1} + b \times \text{CP2}$) is minimised.

i.e. minimise

$$[S - (a \cdot \text{CP1} + b \cdot \text{CP2})] [S - (a \cdot \text{CP1} + b \cdot \text{CP2})] \quad (3)$$

The solution to the problem is simple and is the normal equations ⁽³⁾. The normal equations are used to evaluate polynomial fitting coefficients. Equation 2 has a very similar form to

$$y = a \cdot F_1(x) + b \cdot F_2(x) \quad (4)$$

Which is a two coefficient linear representation of a curve to be fitted to a number of observed data points.

In the case of a straight line fit

$$F_1(x) = 1 \ \& \ F_2(x) = x$$

so that

$$y = a \cdot 1 + b \cdot x$$

In this case the normal linear regression technique would be used to obtain the best fit values for a and b . The general solution to solving for the best match form n compounds to m masses is

$$C = [\text{CP\_MAT}^+ \cdot \text{CP\_MAT}]^{-1} \cdot \text{CP\_MAT}^+ \cdot S \quad (5)$$

Where C is the n dimensional ($n \times 1$) vector representing best fit compositions; S is the $1 \times m$ vector representing the observed spectrum; CP_MAT is a $m \times n$ matrix representing the library cracking patterns. Each of the n rows of CP_MAT are the cracking patterns of the n library compounds used in the fit. CP_MAT^+ is the transpose of CP_MAT .

The values C are then reported as the quantitative amounts.

It is important to note that the fractions a and b must lie in the range (0-1). The regression technique used constrains the parameters to lie in this range ⁽⁴⁾.

Having determined the quantitative amounts, the software then passes on to its statistical validation. This third phase can be eliminated by setting the validation factor to 0 (see section 6.4.4.7.).

The method used is as described in ⁽⁵⁾. If during the regression calculation we have determined the quantitative amounts of n compounds using m masses then we can carry out the following procedure.

Calculate SQ for n compounds = SQ_n. Remove the a compound and recalculate the regression giving a new residual sums of squares SQ_{n-1}. We then calculate the value F from

$$F = \frac{SQ_{n-1} - SQ_n}{SQ_n / (m-n)} \quad (6)$$

We can see that if the gas compound makes up a significant proportion of the mix SQ_{n-1} will be very much larger than SQ_n worse fit giving a large F value. Conversely if removing the compound has very little effect on the sums of squares then SQ_{n-1} $\simeq$ SQ_n giving a low F value.

The value of F obeys an F distribution with 1 and m-n degrees of freedom.. The software successively removes each compound from the fit, starting with the smallest quantity and concluding at the largest quantity. After each removal the statistic F in equation 6 is calculated. This computed value is then compared with the appropriate percentile point (selected in 6.4.4.7.) of the F distribution F (1, n-m) and if greater then the compound is deemed to be present.

References

- 1) Statistics for Physicists BR Martins Academic Press Pg 10
- 2) DD Tunnicliff PA Wadsworth Analytical Chemistry 45.1 Pg 12-20
- 3) Statistics for Physicists BR Martin Academic Press Pg 89
- 4) Statistics for Physicists BR Martins Academic Press Pg 94
- 5) Statistics for Physicists BR Martins Academic Press Pg 93

15. APPENDIX F - REMOTE OPERATION

INTRODUCTION

The purpose of this option is to enable a host computer or serial terminal to remotely control the mass spectrometer i.e. to set mass spectrometer parameters and acquire data.

The distance between the mass spectrometer and the host computer can be up to 30 m, for 9600 baud. This can be extended to many kilometres by using a fibre optic hardware option - this may also be useful in particularly noisy environments.

COMMUNICATIONS PROTOCOL

The communications protocol is referred to as VG CP (VG Communications Protocol).

Remote communications between host computer and the mass spectrometer can be likened to a conversation between two people. Like all good dialogue it is best if only one person speaks at any one time. The initiator of the dialogue obtains a response from the other participant and so on. The host computer **always initiates** dialogue by sending a command, the mass spectrometer **always replies** with a response.

COMMANDS AND RESPONSES

Commands and responses are composed of ASCII alphanumeric character fields separated by a semi-colon (;) and terminated by line-feed and carriage return (<lf> <cr>). Note that characters within a field are case sensitive - **P** does not have the same meaning as **p**

;	Field separator
<lf>	Line-feed character i.e. Ctrl J
<cr>	Carriage return character i.e. Ctrl M

The first field value of all commands and responses, usually a single ASCII character, refers to a command/response type (CR type) which may or may not have additional fields. A list of command/response types is given in appendix I.

Example:-

Host:	O;1<lf><cr>	Commence MIM run
MS:	OK<lf><cr>	Data accepted
Host:	T<lf><cr>	Terminate run i.e.stop MIM run
MS:	RUN TERMINATED<lf><cr>	

PARAMETER CLASSES

There are four types of parameter class under VG CP. These are scalars, arrays of scalars, structures and arrays of structures.

SCALARS

A scalar is a single alphanumeric entity and can be either a:-

Single letter or group of letters, e.g. Y, Methane

Integer number, e.g. 28, 4

Floating point numbers, e.g. 1.32, 4.01 E-7

They refer to either a parameter code or a parameter value and are requested, set and returned by command types. The general command/response is of the form:-

<CR type>;[<Parameter code>;<Parameter value>]]<lf><cr>

A list of parameter codes is given in appendix II.

Example:-

Host: **P;80;30<lf><cr>** Set parameter code 80 to parameter value 30,
i.e. MIM cycles = 30

MS: **OK<lf><cr>** Data accepted

ARRAYS OF SCALARS

This parameter class denotes a number of identical scalar types e.g. integer numbers.

The general command, response form is

**<CR type>;<Parameter code>;<Parameter value 1>;<Parameter value 2>;
<Parameter value n><lf><cr>**

Note: A single parameter code denotes the parameter type for the whole array.

Sometimes the array message may exceed the maximum message length (128 characters). To overcome this the message is broken down into a number of segments. The response message from a get array of scalars command may take the form

**P;<Parameter code>;<Parameter value 1>; ... <lf><cr>
P;<Parameter code>;<Parameter value n>; ... <lf><cr>**

**P;<Parameter code>;<Parameter value r>; ... <lf><cr>
Q;<Parameter code>;<Parameter value n>; .. <lf><cr>**

CR type **P** denotes that the data is incomplete whereas **Q** indicates that it is complete. When the whole array message is short (for example when acquiring a histogram scan over a small mass range) just the **Q** CR type appears. Similarly when setting large arrays CR types '**r**' and '**a**' are used to indicate not complete and complete respectively.

STRUCTURES

This parameter class denotes a mixture of different scalar types e.g. integer numbers and floating point numbers. The general form of the command/response is:-

```
<CR type>;<Parameter code>; <Structure parameter code>;<Structure value>;  
<Structure parameter code>; <Structure value></f></cr>
```

Note: The structure parameter code and its parameter values are sent in pairs thus allowing structures to be sent in any order unlike arrays of scalars which are position dependant.

Example:-

Host: @;151<lf><cr> Get parameter value for parameter code 151
i.e. get MIM data

MS: ^;1.99F-7;2;4.07F-8;17;3;18;300<lf><cr>

Valid request returning complete structure for parameter code 151 (MIM data)

Refer to Section 3 to decode this structure.

As with arrays of scalars, structure messages may be broken down into segments using the CR types p,q,', and ^ . (See Appendix I for details).

ARRAYS OF STRUCTURES

This parameter class denotes an array of identical structures e.g. entries in a MIM recipe.

The general command/response is of the form:

<CR type>;<Parameter code>; <Structure 1>;<Structure n><lf><cr>

Structure n has the form

**<Structure parameter code>; < Structure value>; <Structure parameter code>;
<Structure value>**

Note: That the structures within the array are order dependent.

Example:-

Host:s;10;1;1;2;Y;3;F;4;28;5;Nitrogen;6;2;7;A;8;07;9;1.00;10;N<lf><cr>

MS: OK <lf><cr>

Set array of structures, array incomplete, for parameter code 10,
i.e. set an entry in the MIM recipe.

Again messages can be broken down using the CR types **b**, **c**, **d**, **r**, **s** and **t**.

GETTING STARTED

The power up RS232 configuration of the mass spectrometer is set to 9600 baud, eight data bits, no parity and one stop bit. The host computer or serial terminal, should be set accordingly. Appendix III gives the pin out details of the RS232 port.

If for some reason the host computers RS232 cannot be set to these conditions then the Sensorlab configuration can be altered as described in Appendix IV.

REMOTE OPERATION

To establish the communications link use the pin-pin ribbon cable and null-modem supplied to link between the serial port (COM1) of the mass spectrometer and the RS232 port of the host computer or serial terminal. Start the mass spectrometer in the normal way.

Invoke remote operation by selecting the remote option from the appropriate menu.

Communications should have now been established and the mass spectrometer will wait for a command. If communications are not established correctly check that the host computer is set to the correct baud rate etc and that the RS232 wiring is correct.

Example:-

Host:	P;82;Y<lf><cr>	Set parameter code 82 to Y select pre-locking in MIM
MS:	OK<lf><cr>	Data accepted

To exit from remote operation the X parameter code is used, the computer will revert to the menu

Example:-

Host: X<lf><cr> Exit Remote Control

MS: (there is no reply)

ERROR MESSAGES

On receiving an incorrect command the mass spectrometer replies with one, or more, error messages as shown in the example below.

Host: p<lf><cr> i.e. an incorrect command type

MS: ERROR;UNKNOWN COMMAND <lf><cr>

Host: 0;<lf><cr> i.e. the parameter code had been omitted

MS: ERROR;PARAMETER CODE FORMAT <lf><cr>

Host: P;82;34 <lf><cr> i.e. incorrect parameter value

MS: ERROR;PARAMETER SHOULD BE Y OR N <lf><cr>

Host: s;10;1;1;2;Y;3;N;4;28<lf><cr> i.e. an incorrect parameter
value for structure parameter
code 3

MS: ERROR;10;3;PARAMETER SHOULD BE M, F OR U <lf><cr>

USING MIM MODE REMOTELY

In MIM mode the host computer or serial terminal can:-

- Set cycle times, pre-locking etc
- Set up the recipe
- Run MIM and receive data
- Set alarm limits

CYCLE TIMES, PRE-LOCKING ETC

Parameter code 80 sets up the number of cycles MIM will run for.

Example:-

Host: **P;80;30 <lf><cr>** Set 30 cycles limit

MS: **OK<lf><cr>** Data accepted

The time period between cycles can be set using parameter code 83. The mass spectrometer measures time in units of 0.1 seconds. Thus to set a 5 second time period between cycles we need to specify 50 mass spectrometer time units.

Example:-

Host: **P;83;50<lf><cr>** Set time period to 5 secs

MS: **OK<lf><cr>** Data accepted

Pre-peak locking, refer to mass spectrometer manual for an explanation of this term, is set using parameter code 82.

Example:-

Host: **P;82;N<lf><cr>** No pre-locking

MS: **OK<lf><cr>** Data accepted

Pre zeroing, refer to mass spectrometer manual for an explanation, is set using parameter code 85.

Host: P;85;Y<lf><cr> Enable Pre Zeroing

MS: OK<lf><cr> Data accepted

Alarm checking, refer to mass spectrometer manual for an explanation, is set using parameter code 84

HOST: P;84;N <lf><cr> Disable Alarms

MS: OK<lf><cr> Data accepted

Alarm units, refer to mass spectrometer manual for an explanation, are selected to parameter code 86

HOST: P;86;Y <lf><cr> Alarm values in partial pressure units

MS: OK<lf><cr> Data accepted

HOST: P;86;N <lf><cr> Alarm values in percent

MS: OK <lf><cr> Data accepted

SETTING A RECIPE

The MIM mode recipe is set using parameter code 10 - an array of structures. Each structure represents a single channel in the MIM recipe. Table 1 shows how each structure is composed.

Example:-

Host: s;10;1;1;2;Y;3;F;4;28;5;Nitrogen;6;2;7;A;8;7;9;1.00;10;N;11;0.0e-10;12;9.999e-5<lf><cr>

MS: OK<lf><cr>

Set channel 1 to measure Nitrogen using the Faraday detector with auto-ranging, no storage required. Note the array of structures is incomplete, as indicated by the s command type.

Example:-

Host: t;10;1;4;2;Y;3;M;4;40;5;Argon;6;2;7;A;8; 9;9;1.00;10;N;
 11;0.0;12;5.4e-5<lf><cr>

MS: OK<lf><cr>

Set channel 4 to Argon using the multiplier detector with fixed gain M-9, no storage required. Note the array of structures is complete, i.e. the whole recipe is complete, as indicated by the t command type.

Structure Parameter Code	Item	Type	Example	Limits
1	Channel Number	numeric	01	1-16
2	Channel Enabled	alpha	Y	Y or N
3	Detector Type	alpha	F	F, M or U
4	Mass	numeric	104	0-999
5	Name	alphanumeric	10	Methane
6	Accuracy Code	numeric	2	1,2,3 or 4
7	Autoranging	alpha	A	A or C
8	Gain Range	numeric	7	5-13
9	Relative Sensitivity	numeric	1.02	0.01-100.00
10	Store	NOT USED remotely		
11	Low Alarm	numeric	1.7e-7	0.0-9.99e-5 or 0.0-100.0
12	High Alarm	numeric	27.34	0.0-9.99e-5 or 0.0-100.0

TABLE 1

MIM Recipe, Array of Structures, Parameter Code 10

(Setable Only)

Footnote: The limits on low/high alarms depends on the alarm mode selected.

RUNNING MIM

Once all the relevant parameters have been set MIM mode is run using parameter code O.

Example:-

```
Host:      O;1<lf><cr>      Run MIM
MS:        OK<lf><cr>      Data accepted
```

To acquire data from the computer the parameter code @ is used.

Example:-

```
Host:      @;151<lf><cr>    Request MIM data
MS:        ^;151;1;1.99F-7;2;4.07F-8;17;3;18;300<lf><cr>
```

The data returned is in the form of a structure. Structure parameter codes 1-16 refer to channel numbers - the structure parameter value is the partial pressure associated with that channel.

Structure parameter code 17 gives the cycle number and structure parameter code 18 gives the time in one tenth second units from the start of a run. This number ranges from 0 to 864000 (24 x 60 x 60 x 10). So in the above example the data is for cycle number 3 and was taken 30 secs into the run.

To terminate the run parameter code T is used.

Example:-

```
Host:      T<lf><cr>      Terminate run
MS:        RUN TERMINATED<lf><cr>
```

REMOTE SCAN MODE ACCESS

All of the scan modes may be controlled remotely - analogue scan; histogram scan and logarithmic histogram scan.

Scan definition structure

The scan parameters are defined by structure number 131. Details of the structure members are given in Table 2.

Structure Parameter Code	Item	Type	Example	Limits
1	Detector Type	alpha	F	F or M
2	Start gain	numeric	7	5-10 (Faraday) 7-13 (Sem)
3	End gain	numeric	6	5-10 (Faraday) 7-13 (Sem)
4	Start mass amu	numeric	01	0-maximum mass
5	End mass amu	numeric	200	0-maximum mass
6	Averaging	numeric	300	1-4096

TABLE 2
Scan Parameter Structure Code 131 (Setable only)

Note that the End gain is only used for logarithmic scan, also the averaging is only used by analogue and histogram scan.

GETTING SCAN INFORMATION

Scan information is sent back in two segments. The first segment is a structure (code 156) defining the scan parameters (time etc.). The second segment is the body of the scan values; this is sent as an array of scalars. The array of scalars is sent back in segments (using the P and Q first field identifiers). This is done to limit the message length to 128 characters.

Overleaf flow chart 1 demonstrates how to obtain an analogue scan.

SCAN PREAMBLE STRUCTURE

Table 3 shows the scan preamble structure.

Structure Parameter Code	Item	Type	Example	Limits
1	Scan Time in 1/10 seconds	numeric	3000	0-864000
2	Start mass	numeric	10	0-maximum mass
3	End mass	numeric	200	0-maximum mass
4	Status OK	alpha	Y	Y or N

TABLE 3

Scan preamble structure 156 (Readable Only)

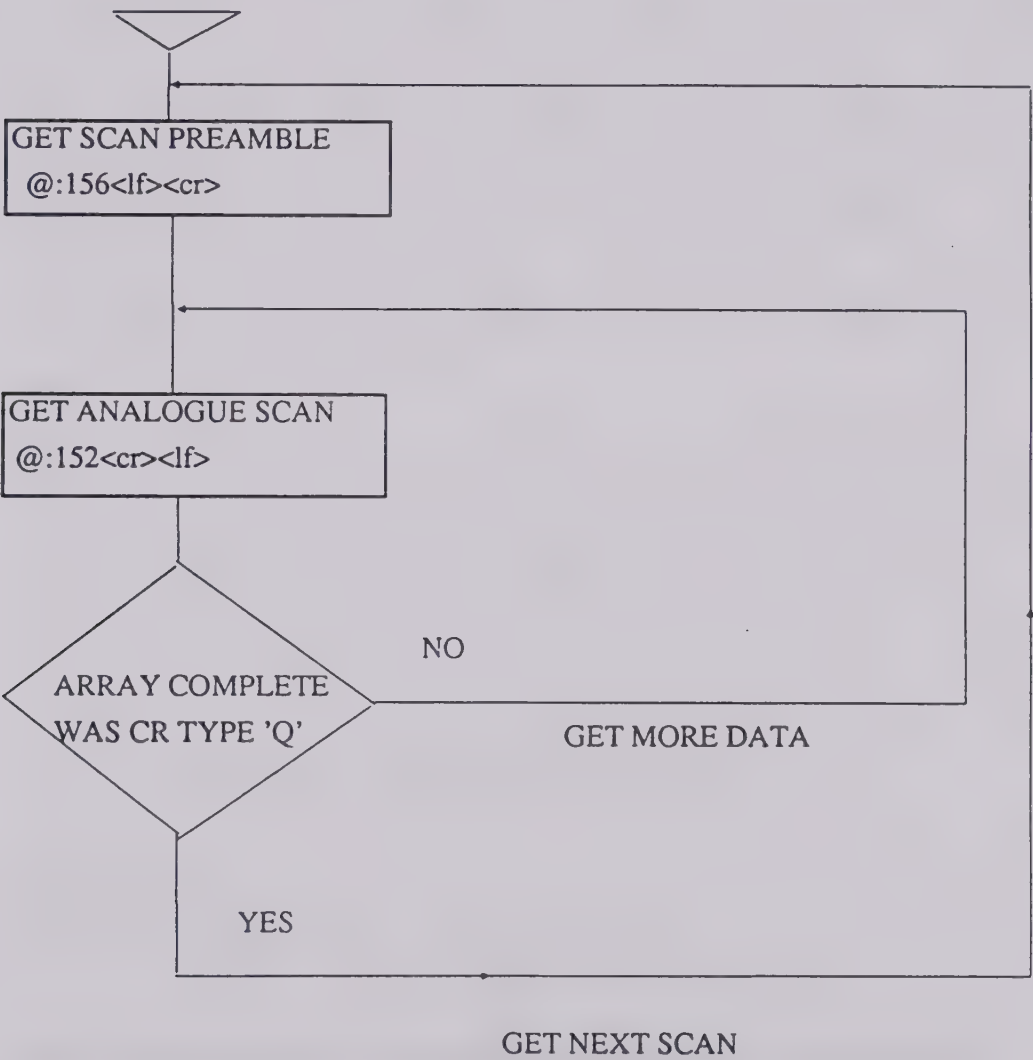
typical response is: ^;156;1;100;2;4;3;189;4;Y <lf><cr>
indicates a time of 10 seconds, start mass of 4, end mass of 189 and status OK.

SCAN VALUES

Scan values are sent back in VG signal value format, best demonstrated by the following example.

```
P;153;1.1F-10;2.3F-10;7.0F-7<lf><cr>
```

Note that for analogue and histogram scan the gain values will be the same for all readings.



Flow Chart 1 - getting scan data

REMOTE MASS ALIGNMENT**SCAN DEFINITION STRUCTURE**

The mass alignment parameters are defined by structure number 130. Details of the structure members are given in Table 4.

Structure Parameter Code	Item	Type	Example	Limits
1	Detector Type	alpha	F	F or M
2	Start gain	numeric	6	5-10 (Faraday) 7-13 (Sem)
3	End gain	numeric	7	5-10 (Faraday) 7-13 (Sem)
4	Start mass amu	numeric	01	0-maximum mass
5	End mass amu	numeric	200	0-maximum mass
6	Search Mode	alpha	I	E (Existing) I (Ideal)

TABLE 4

Histogram Mass Alignment Parameter Structure Code 130 (Setable only)

SETTING COMMAND PAGE VARIABLES

EMISSION AND FILAMENT

Command page variables (except SEM) can be set from the command page structure (number 132).

Table 5 shows the structure items.

Structure Parameter Code	Item	Type	Example	Limits
1	Emission	alpha	Y	Y or N
2	Filament	numeric	1	1 or 2

TABLE 5

Command page structure parameter code 132 (setable only)

eg: q;132;1;Y;2;1<lf><cr>
turns emission on and selects filament 1.

SEM

SEM values are set from the SEM structure (number 110).

Table 6 Shows the structure items.

Structure Parameter Code	Item	Type	Example	Limits
1	SEM ON	alpha	Y	Y or N
2	Volts	numeric	1200	600-3500
3	Calibration mass	numeric	28	0-maximum mass
4	Calibrate	alpha	Y	Y or N

TABLE 6

SEM structure parameter code 110 (Setable only)

eg : q; 110; 1;Y;2;1000;4;N <lf><cr>

turns SEM on at 1500 volts with no auto calibrate

PARAMETER ACCESS MODES

Parameter access modes affect the data format. At the moment access formats can be changed for the following parameters.

151	Acquire	MIM Data
152	Acquire	Analogue Scan Data
153	Acquire	Histogram Scan Data
154	Acquire	Log Histogram Scan Data
156	Acquire	Scan Preamble

There are two access modes available

- Access Mode 1 - Transmit data without checksum
- Access Mode 2 - Transmit data with checksum appended

To set Log Histogram Scan Data to checksum access mode:-

```
R;154;2 <lf><cr>
```

Parameter access modes can be acquired using the S CR type. For example after the above command

```
S;154 <lf><cr>
```

Produces the response

```
I;151;2 <cr><lf>
```

Indicating that MIM data will have a checksum appended

Checksums are evaluated as follows:-

All ASCII values of the message (excluding the <lf><cr> are summed. 64 decimal is added to the sum modulo 64.

eg $Checksum = 64 + (\sum ASCII\ CODES \% 64)$
where % represents the modulo operator eg $125 \% 64 = 61$

For host computers that do not have a modulo arithmetic operator modulo 64 can be achieved by adding the sum of ASCII codes with hexadecimal 3F.

eg Checksum = 64 + ($\sum$ ASCII CODES 'AND' HEX3F)

The checksum is the last message character before the <lf><cr>.

If the host machine detects a checksum error then there is no mechanism for re-accessing the data - the data is best discarded.

All access modes are defaulted to 1 on power up.

APPENDIX I**VG CP Command/Response Types**

<u>Commands</u>	<u>ASCII characters</u>	<u>Example</u>
Commence Run	O	O;1<lf><cr> go MIM
Halt Run	T	T<lf><cr>
Exit Remote Operation	X	X<lf><cr>
Get Parameter	@	@;156<lf><cr> get scan preamble
Set Scalar	P	P;80;27<lf><cr> set MIM CYCLES to 27
Set Array of Scalars Array Incomplete	,	Currently not used
Set Array of Scalars Array Complete	a	Currently not used
Set Structure Structure Incomplete	p	P;110;1;7;2;1500<lf><cr>SEM- on 1500 volts
Set Structure Structure Complete	q	q;110;3;40;4;7<lf><cr>SEM calibrate at mass 40 amu
Set of Array of Structures Structure Incomplete	r	r;10;1;3;6;3<lf><cr> MIM channel 3 accuracy code to 3
Set Array of Structures Structure Complete	s	s;10;1;3;12;7.4e-7 MIM channel 3 high alarm limit to 7.4e-7
Set Array of Structures Array and Structure Array	t	t;10;1;16;12;7.4e-7 MIM channel 16 high alarm limit to 7.4e-7
Set Parameter Access Mode	R	R;154;2 <lf><cr>set checksum on for log hist data
Get Parameter Access Mode	S	S;154<lf><cr> get current access mode for log hist data

Responses

	ASCII Characters	Example
Data Accepted	OK	
Error	ERROR	ERROR;82;PARAMETER SHOULD BE Y OR N<lf><cr>
System Busy	BUSY	
Valid Request Returning Scalar	@	Currently not used
Valid Request Returning Array of Scalars - Array Incomplete	P	P;154;7.1F-7;0.1F-10 <lf><cr> log hist data returned array incomplete
Valid Request Returning Array of Scalars - Array Complete	Q	Q;154;0.01F-10;0.03F-10<lf><cr> log hist data returned array complete
Valid Request Returning Structure - Structure Incomplete	,	Currently not used
Valid Request Returning Structure - Structure Complete	^	^;156;1;100;2;4;3;189;4;Y<lf><cr> returning scan preamble
Valid Request Returning Array of Structures - Structure Incomplete	b	Currently not used
Valid Request Returning Array of Structures - Structure Complete	c	Currently not used
Valid Request Returning Array of Structures - Structure and Array of Structures Complete	d	Currently not used
Valid Request Returning Parameter Access Mode	I	Currently not used

APPENDIX II**VG CP Parameter Codes**

Start Multiple Ion Monitoring (MIM)	1
Start Analogue Scan	2
Start Histogram Scan	3
Start Histogram Mass Alignment	4
Start Log Histogram Scan	5
Define MIM Recipe	10
Define number of MIM cycles	80
Define Multiplexer Channel Number	81
Define MIM Pre-Lock Status	82
Define MIM Cycle Period	83
Enable/Disable Alarms in MIM	84
Define MIM Pre Zero Status	85
Alarm units	86
Define SEM Parameters	110
Define Mass Alignment Parameters	130
Define Scan Parameters	131
Set Command Page Variables	132
Acquire MIM Data	151
Acquire Analogue Scan Data	152
Acquire Histogram Scan Data	153
Acquire Log Histogram Scan Data	154
Acquire Scan Preamble	156

APPENDIX III

Serial Port options on IBM PC's and Compatibles used as a Mass Spectrometer Controller.

Two options a) 9-pin D-Shell RS232C port

 b) 25-pin D-Shell RS232C port

when option a) is fitted with an optional IBM communications cable, which has a 9-pin D-Shell connector on one end and a 25-Pin D-Shell connector on the other end, the 25-Pin end of the cable has all of the signals of a standard EIA RS232C.

Pin Assignments for 9-way D-Type Connector

	Description	Pin	
External Device	Carrier Detect	1	Serial
	Receive Data	2	Adaptor
	Transmit Data	3	in mass
	Data Terminal Ready	4	Spectrometer
	Signal Ground	5	
	Data Set Ready	6	
	Request To Send	7	
	Clear To Send	8	
	Ring Indicator	9	

Pin Assignment for 25 way D-Type Connector

Description		Pin	
External Device	NC	1	Asynchronous Communications Adapter (RS232C) in mass Spectrometer
	Transmitted Data	2	
	Received Data1	3	
	Request to Send	4	
	Clear to Send	5	
	Data Set Ready	6	
	Signal Ground	7	
	-Receive		
	Line Signal Detector	8	
	Transmit		
	Current Loop Data	9	
	NC	10	
	Transmit		
	Current Loop Data	11	
	NC	12	
	NC	13	
	NC	14	
	NC	15	
	NC	16	
	NC	17	
	+Receive		
	Current Loop Data	18	
	NC	19	
	Data Terminal Ready	20	
	NC	21	
	Ring Indicator	22	
	NC	23	
	NC	24	
	-Receive		
	Current Loop Return	25	

APPENDIX IV

Altering the RS232 presets

In order to perform this function with Micromass you will need access to an IBM PC or compatible. It must have one floppy disk drive the same as on your Micromass i.e. if you have a 5 1/4 inch floppy disk on your Micromass your PC must have a 5 1/4 inch drive. To change RS232 presets you will need to edit line 1 of the config.sys file. As supplied line 1 will read

```
device = com.sys 9600,n,8,1
```

This indicates 9600 baud, no parity, 8 data bits and 1 stop bit. Usually the best way to edit this line is to use the PC/MS DOS line editor EDLIN. For Spectralab users with hard disks EDLIN will be found in the \PCDOS directory for an IBM PC or the MSDOS subdirectory for compatibles.

Change to this directory and type

```
EDLIN \CONFIG.SYS
```

Details on how to use EDLIN are contained in the PCDOS technical manual.

Alteration of RS232 presets is best demonstrated by examples

```
device = comml.sys 4800,e,7,1
```

sets 4800 baud, even parity, 7 data bits and 1 stop bit

```
device = comml.sys 1200, n, 8,1
```

sets 1200 baud, no parity, 8 data bits and 1 stop bit

The format of the line is identical to the **mode com 1** = command under PC/MSDOS.

APPENDIX V - EXAMPLE BASIC PROGRAM LISTING

```
10 ' VG Quadrupoles Limited Software
20 ' Remote Control Test Program - Histogram Scan Run
30 ' software written in gwbasic
40 ' responses from the mass spec are displayed but are not
50 ' tested for correctness
60 ' check sums incorporated and checked, if unmatched remote exited
70 '
80 CLS
90 PRINT "REMOTE CONTROL TEST PROGRAM"
100 PRINT "HISTOGRAM SCAN RUN"
110 '
120 ' initialise RS232 port
130 OPEN "COM1:9600,N,8,1" AS #1
140 '
150 ' setup variables with dummy values for entry into input routines
160 SMASS=1000:EMASS=1000:SGAIN=0
170 DET$="-":NLINE$=CHR$(10)+CHR$(13)
180 '
190 ' input routines for histogram scan parameters
200 '
210 WHILE DET$<>"F" AND DET$<>"M"
220 PRINT"ENTER THE DETECTOR TYPE (F, M) ";
230 DET$=INPUT$(1):PRINT DET$
240 WEND
250 WHILE ((SGAIN <6 OR SGAIN >9) AND DET$="F") OR ((SGAIN <7 OR SGAIN >13) b
    AND DET$="M"
260 PRINT"ENTER THE GAIN RANGE (6-9 FOR F, 7-13 FOR M) ";
270 INPUT SGAIN
280 WEND
290 WHILE SMASS <0 OR SMASS>200
300 PRINT"ENTER THE START MASS (0-200) ";
310 INPUT SMASS
320 WEND
330 WHILE EMASS<0 OR EMASS>200
```

```
340 PRINT"ENTER THE END MASS (0-200) ";
350INPUT EMASS
360 WEND
370 '
380 ' send setup parameters for histogram scan
390PRINT#1,"q;131;1;" +DET$+";2;" +STR$(SGAIN)+";3;" +STR$(SGAIN)+";4;"
    +STR$(SMASS)+";5;" +STR$(EMASS)+NLINES$;
400 GOSUB 740:' get response from Sensorlab
410 '
420 ' send commands for checksum calculations
430 PRINT#1, "R;156;2"+NLINES$;
440 GOSUB 740
450 PRINT#1, "R;153;2"+NLINES$;
460 GOSUB 740
470 PRINT:PRINT"STARTING HISTOGRAM SCAN RUN"
480 '
490 ' start histogram scan run
500 PRINT#1, "O;3"+NLINES$;
510 GOSUB 740:' get response from Sensorlab
520 GOSUB 930:' pause
530 '
540 ' get scan preamble
550 PRINT#1, "@;156"+NLINES$;
560 GOSUB 740:' get response from Sensorlab
570 GOSUB 1110:' get checksum
580 GOSUB 930:' pause
590 '
600 ' get scan values
610 PRINT#1, "@;153"+NLINES$;
620 GOSUB 740:' get response from Sensorlab
630 GOSUB 1110:' get checksum
640 '
650 ' test for more scan values to be read
660 IF MID$(RES$,1,1)="P" THEN GOTO 600
670 '
680 ' if X from keyboard exit remote
```

```
690 FOR I=0 TO 500:IF INKEY$="X" THEN GOTO 980:NEXT I
700 '
710 ' get next scan preamble
720 GOTO 520
730 END
740 '
750 ' read string of output from Sensorlab
760 '
770 GOSUB 880:' read 1 character from Sensorlab
780 RES$=ANS$
790 CHAR=ASC(ANS$)
800 ' test for carriage return for end of string
810 WHILE CHAR<>10
820   PRINT ANS$;
830   GOSUB 880:' read 1 character from Sensorlab
840   CHAR=ASC(ANS$)
850   RES$=RES$+ANS$
860 WEND
870 RETURN
880 '
890 ' read one character from Sensorlab
900 '
910 ANS$=INPUT$(1,#1)
920 RETURN
930 '
940 ' delay loop for RS232 control
950 '
960 FOR I=0 TO 8000:NEXT I
970 RETURN
980 '
990 ' exit remote histogram scan mode
1000 '
1010 GOSUB 930:' pause
1020 ' terminate run
1030 PRINT#1, "T"+NLINES$
1040 GOSUB 740:' get response from Sensorlab
```

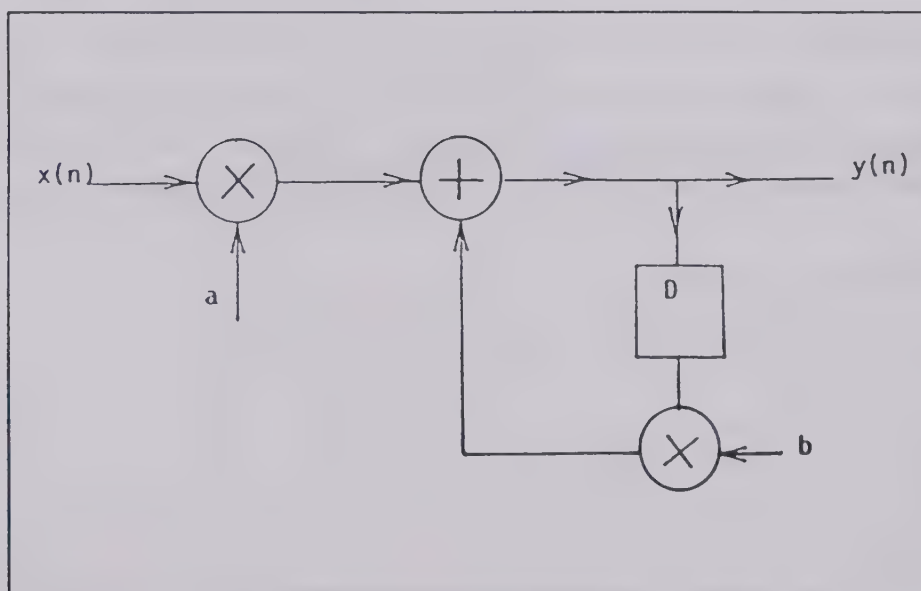
```
1050 GOSUB 930:' pause
1060 '
1070 ' exit from remote system
1080 PRINT#1, "X"+NLINES$
1090 PRINT:PRINT"EXITING REMOTE SYSTEM"
1100 END
1110 '
1120 ' calculate checksum
1130 '
1140 CHECK=0
1150 FOR I=1 TO LEN(RES$)-3
1160   CHECK=CHECK+ASC(MID$(RES$,I,1))
1170 NEXT I
1180 CHECK=(CHECK MOD 64)+64
1190 IF ASC(MID$(RES$,LEN(RES$)-2,1))<>CHECK THEN GOTO 1210
1200 RETURN
1210 '
1220 ' checksum error
1230 '
1240 PRINT:PRINT"ERROR CHECKSUMS UNMATCHED"
1250 GOTO 980
1260 END
```

16. APPENDIX G - DIGITAL FILTERING

A digital filter accepts as its input a stream of discrete signal values. These signal values are modified according to a specific algorithm to produce a stream of output values. These digital values could be produced by an analog to digital convertor that is sampling a continuous signal. According to the sampling theory the sample rate should be at least twice the highest frequency component present in the continuous signal. In contrast an analog filter deals with continuous signals only i.e. signals that are defined at all points in time.

In Analog scan mode, 600 readings are taken over the user selected mass range. Thus an analog scan is a stream of discrete digital values. The digital filter is designed to model a second order low pass Butterworth filter. The attenuation of the filter is strongest for signals that are less than the width of one peak i.e. less than one amu. Note that the filter will accept any low frequency periodic noise where as averaging will cancel it out.

The algorithms for digital filters are derived using Z-Transforms, a discrete form of Laplace Transform. Although the use of Z-Transforms can be quite complex the resulting algorithm is very simple indeed. The output of the digital filter simply depends upon present and previous inputs and outputs.



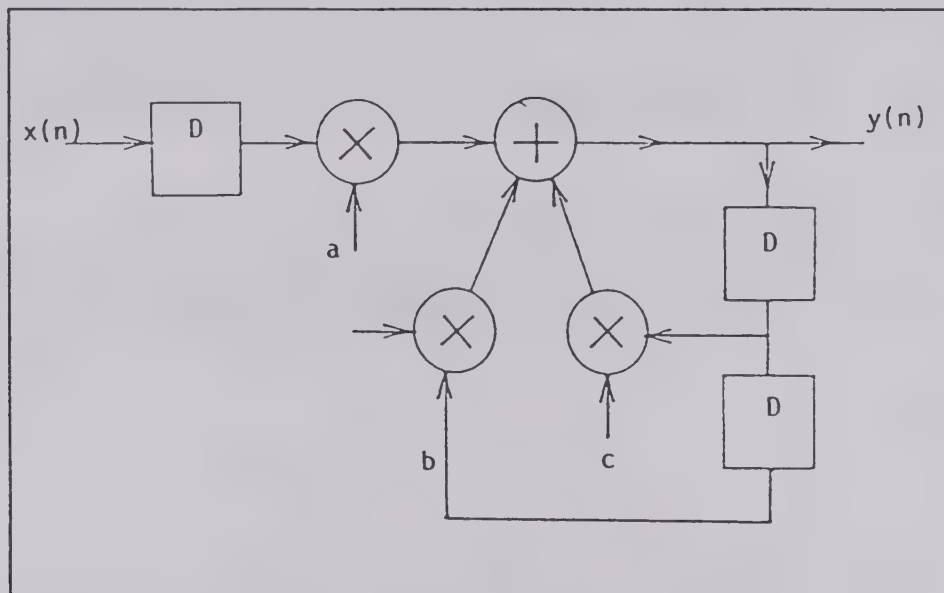
A simple first order low pass filter can be represented by the above diagram.

$$y(n) = a.x(n) + b.y(n-1)$$

Thus it can be seen that the output of the filter, $y(n)$, depends upon the present input, $x(n)$, and the previous output, $y(n-1)$. 'D' is a unit delay, 'a' and 'b' are multiplication factors, and 'n' is a discrete point in time, the sample time.

A filter that depends upon previous outputs is sometimes known as a recursive or infinite impulse response (IIR) filter. Non-recursive filters depends upon previous inputs only.

The filter incorporated into Analog scan can be represented by the following diagram.



The equivalent equation is:-

$$y(n) = a.y(n-1) + b.y(n-2) + c.x(n-1)$$

The coefficients are given by:-

$$a = 2.\cos(\text{var}).\exp(-\text{var})$$

$$b = -(\exp(-\text{var}))^2$$

$$c = \text{cut\_off}.\sqrt{2}.\sin(\text{var}).\exp(-\text{var})$$

$$\text{Where } \text{var} = \text{cut\_off} \times 0.02/\sqrt{2}$$

$$\text{cut\_off} = \text{endmass} - \text{startmass}$$

Endmass and startmass correspond to the user selected mass range for the analogue scan. The value of cut_off is limited to less than 100.

The filter also requires a normalisation factor. This is required to give a unit gain at frequencies less than the cut off point of the filter. Thus

$$y'(n) = y(n)/\text{norm}$$

$$\text{where norm} = c/(1-a-b)$$

Most analog filters have a phase delay between input and output and this is true of digital filter also. In Analogue scan this phase delay has been allowed for. Although, at very small mass ranges (a few amu) a very small peak shift may be perceived when digital filtering is switched on.

If you have the binary to ASCII data file converter program, **DATA CONVERSION**, then note the following. Analogue scan files that are stored with the digital filtering option on will be stored with NREADINGS set to 2048. The actual number of readings per point is one. The number 2048 is merely used as a 'signature' for digital filtering. NREADINGS is the 9th item in a data file header.

REFERENCES

"Continuous and Discrete Signal and System Analysis", C D McGillem, G R Cooper
CBS College Publishing
Chapter 6, "The Z-Transform and Digital Filters"

Calibration

a) **Case where principal mass peaks do not overlap - using MIM**

As mentioned in Appendix D gases have different ionisation efficiencies. Although Appendix D gives a way of calculating the relative ionisation efficiencies it is recommended that they are determined on your specific quadrupole using calibration. It is conventional to base ionisation efficiencies on that of Nitrogen, although any gas could be used. The calculation of relative ionisation efficiencies is best demonstrated by an example. For instance let us assume that a gas mixture of O₂ (mass 32); N₂ (mass 28); Ar (mass 40) is to be measured. Let us further assume that we have a calibration mixture of 35%N₂; 25%O₂; 40%Ar. We infuse the calibration mixture into the mass spectrometer, for those with gas monitoring just place the inlet capillary into the calibration gas stream. We then measure the peak heights at mass 28 (N₂); mass 32 (O₂) and mass 40 (Ar) using an, autorange measurement in MIM - all measurements should be performed on the same detector and all relative efficiencies should be set to 1. The relative ionisation efficiencies based on N₂ are calculated as follows:

Relative ionisation efficiency N2 = 1.0

$$\text{Relative ionisation efficiency O}_2 = \frac{\text{mass 32 peak height} / 25}{\text{mass 28 peak height} / 35}$$

$$\text{Relative ionisation efficiency Ar} = \frac{\text{mass 40 peak height} / 40}{\text{mass 28 peak height} / 35}$$

These values should be entered into the relative efficiency column in the MIM recipe. To determine unknown percentages of the gases N₂, O₂ & Ar infuse the mixture into the mass spectrometer run MIM and select percentage mode.

b) **Overlapping principle mass peaks using log library**

With Quasar software it is possible to calculate mixtures of gases whose principal peaks overlap using the log library regression software (described in Appendix E)

In order for the regression technique to work successfully the cracking pattern of each gas must be determined. The best way of doing this is to infuse each gas into the mass spectrometer and enter the cracking pattern into the library data base.

Again the technique will be explained by an example of the gases N2, CO and CO2

MASS	12	13	14	16	28	29	30	44
Gas N2	-	-	5.2	-	100.0	0.7	-	-
CO	4.7	0.1	0.8	1.7	100.0	-	0.2	-
CO2	6.7	0.9	-	9.4	8.2	1.0	-	100.0

TABLE 1

Table 1 shows the cracking pattern for each gas, there are a large number of mass overlaps. The recommended calibration procedure would be as follows:

Infuse 100% N2 into the system run log histogram scan over 3 decades with mass 28 (principle peak) contained in the least sensitive decade. Note the peak height of mass 28 (using the mass cursor on 28) Enter library and select option 5 - store current scan into library - you will then be presented with the normal cracking pattern edit page (6.4.4.3.). You should remove any small noise peaks found - ie. masses not in table 1 - by overwriting the intensities with 0. This procedure should be repeated with 100% CO and 100% CO2 to establish their cracking pattern.

For each gas you should enter the following values in the relative sensitivity field (relative ionisation efficiency) while editing the cracking pattern.

N2	enter	-1.0
CO	enter	<u>Peak height of mass 28 for 100% CO</u> Peak height of mass 28 for 100% N2
CO2	enter	<u>peak height of mass 44 for 100% CO2</u> Peak height of mass 28 for 100% N2

Finally you should set up a group containing N₂, CO and CO₂ using the edit group facility described on (6.4.4.4). To determine amounts of the 3 gases in unknown mixtures run as a 3 decade log histogram (most intense peak contained in least sensitive decade) enter log library and invoke the automatic search (option 1). Select the group containing just the three gases above. The percentage amounts will then be determined using the regression procedure and displayed.

c) Assessment of random and systematic errors from log library regressions.

When using the technique described previously some times errors can occur. The most common cause of errors are systematic errors resulting from improper determination of cracking patterns. For example using a 10% N₂, 90% CO bottle to determine the CO cracking pattern. It is vital that, in order for the procedure to work, cracking patterns must be determined correctly. When considering random errors it is very important to note that although the individual mass measurements have independent errors the errors on the quantitative amounts displayed are not independent. In statistical parlance the determined quantitative amounts have non zero covariances. A comprehensive analysis of errors from regressions is presented in BR Martins book (1). The quantitative amounts variance co variance has a term in it involving

$$[\text{CP.MAT}^T \text{CP.MAT}]$$

Where CP.MAT is the rectangular matrix of cracking patterns described in Appendix E. The greater the mass spectral overlaps the higher the covariance will be. Again the effect of this is best considered by an example. Consider an attempt to measure 1% of CO in the presence of 99% N₂, if the relative error on the N₂ quantitative amount is 1% then this error could introduce an absolute error of 0.9% on the CO determination error giving it a relative error of 90%. The effect would be nothing like as bad for a 1% CO₂, 99% N₂ where the co variance term is much lower.

In general it is not a good idea to try and measure small quantities of gases which overlap strongly with large quantities of gases.

[1] Statistics for Physicists BR Martin Academic Press Pg. 91

18. WARRANTY

Products of VG Quadrupoles Limited are warranted to be free from all defects in material and workmanship. The liability of VG Quadrupoles under this guarantee is limited to servicing, adjusting or replacing defective parts. The guarantee on this basis is effective from the date of despatch to the original purchaser from 12 months provided:

1. The product is returned to the factory transportation charges prepaid and damage has not been caused by failure to provide sufficient packaging.
2. The product appears to VG Quadrupoles satisfaction to be defective through no fault of the user.
3. The guarantee only applies if the equipment is operated in accordance with the instructions and advice detailed in the appropriate operating instruction manual or any other instructions which may be provided by VG Quadrupoles Limited. Mass spectrometer filaments are not included.
4. The guarantee does not apply to components including electron multipliers which are outside the component manufacturers usual guarantee period.

Filaments are classed as consumables, and are not covered by this warranty.

Site visits can be arranged at all times in the instruments life. For equipment under warranty the purchaser must pay for engineers travelling and accommodation (if required) and forward an order number before the visit can take place. For site visits outside the warranty period, contact your Service department for details.

Service contracts are available on most equipment to meet your specific requirements, please contact your local Service Department below for details.

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